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(54) Title: CRYSTALLIZED PPAR$G(A) LIGAND BINDING DOMAIN POLYPEPTIDE AND SCREENING METHODS EMPLOYING SAME

(57) Abstract: A solved three-dimensional crystal structure of a PPARα ligand binding domain polypeptide is disclosed, along with a crystal form of the PPARα ligand binding domain polypeptide. Methods of designing modulators of the biological activity of PPARα and other PPAR ligand binding domain polypeptides are also disclosed.

CRYSTALLIZED PPARα LIGAND BINDING DOMAIN POLYPEPTIDE AND SCREENING METHODS EMPLOYING SAME

Technical Field

The present invention relates generally to the structure of the ligand binding domain of PPARα, and more particularly to the structure of the ligand binding domain of PPARα in complex with a ligand. The invention further relates to methods by which modulators and ligands of PPARα and other PPARs can be identified.

Abbreviations

ATP	adenosine triphosphate
ADP	adenosine diphosphate
BSA	bovine serum albumin
cDNA	complementary DNA
DBD	DNA binding domain
DMSO	dimethyl sulfoxide
DNA	deoxyribonucleic acid
DTT	dithiothreitol
EDTA	ethylenediaminetetraacetic acid
HEPES	N-2-Hydroxyethylpiperazine-N'-2-ethanesulfonic acid
kDa	kilodalton(s)
LBD	ligand binding domain
mPPAR	mouse peroxisome proliferator activated receptor
NDP	nucleotide diphosphate
NTP	nucleotide triphosphate
PAGE	polyacrylamide gel electrophoresis
PCR	polymerase chain reaction
pI	isoelectric point
PPAR	peroxisome proliferator-activated receptor
PPARα	peroxide proliferator-activated receptor alpha

PPRE	PPAR response element
rPPAR	rat peroxisome proliferator activated receptor
RXR	retinoid X receptor
SDS	sodium dodecyl sulfate
SDS-PAGE	sodium dodecyl sulfate polyacrylamide gel electrophoresis

Amino Acid Abbreviations

Single-Letter Code	Three-Letter Code	Name
A	Ala	Alanine
V	Val	Valine
L	Leu	Leucine
I	Ile	Isoleucine
P	Pro	Proline
F	Phe	Phenylalanine
W	Trp	Tryptophan
M	Met	Methionine
G	Gly	Glycine
S	Ser	Serine
T	Thr	Threonine
C	Cys	Cysteine
Y	Tyr	Tyrosine
N	Asn	Asparagine
Q	Gln	Glutamine
D	Asp	Aspartic Acid
E	Glu	Glutamic Acid
K	Lys	Lysine
R	Arg	Arginine
H	His	Histidine

Functionally Equivalent Codons

Amino Acid			Codons
Alanine	Ala	A	GCA GCC GCG GCU
Cysteine	Cys	C	UGC UGU
Aspartic Acid	Asp	D	GAC GAU
Glumatic acid	Glu	E	GAA GAG
Phenylalanine	Phe	F	UUC UUU
Glycine	Gly	G	GGA GGC GGG GGU
Histidine	His	H	CAC CAU
Isoleucine	Ile	I	AUA AUC AUU
Lysine	Lys	K	AAA AAG
Methionine	Met	M	AUG
Asparagine	Asn	N	AAC AAU
Proline	Pro	P	CCA CCC CCG CCU
Glutamine	Gln	Q	CAA CAG
Threonine	Thr	T	ACA ACC ACG ACU
Valine	Val	V	GUA GUC GUG GUU
Tryptophan	Trp	W	UGG
Tyrosine	Tyr	Y	UAC UAU
Leucine	Leu	L	UUA UUG CUA CUC CUG CUU
Arginine	Arg	R	AGA AGG CGA CGC CGG CGU
Serine	Ser	S	ACG AGU UCA UCC UCG UCU

Background Art

Nuclear receptors reside in either the cytoplasm or nucleus of eukaryotic cells and represent a superfamily of proteins that specifically bind a physiologically relevant small molecule, such as a hormone or vitamin. As a result of a molecule binding to a nuclear receptor, the nuclear receptor

changes the ability of a cell to transcribe DNA, i.e. nuclear receptors modulate the transcription of DNA. However, they can also have transcription independent actions.

Unlike integral membrane receptors and membrane-associated receptors, nuclear receptors reside in either the cytoplasm or nucleus of eukaryotic cells. Thus, nuclear receptors comprise a class of intracellular, soluble, ligand-regulated transcription factors. Nuclear receptors include but are not limited to receptors for glucocorticoids, androgens, mineralcorticoids, progestins, estrogens, thyroid hormones, vitamin D, retinoids, icosanoids and pertinently, peroxisome proliferators. Many nuclear receptors, identified by either sequence homology to known receptors (See, e.g., Drewes et al., (1996) *Mol. Cell. Biol.* 16:925-31) or based on their affinity for specific DNA binding sites in gene promoters (See, e.g., Sladek et al., *Genes Dev.* 4:2353-65), have unascertained ligands and are therefore termed "orphan receptors".

Peroxisomes are organelles that are involved in the β-oxidation of long-chain fatty acids and the catabolism of cholesterol to bile acids (See, e.g., Vamecq & Draye, (1989) *Essays Biochem.* 24: 115-225). Peroxisome proliferators are a structurally diverse group of compounds which, when administered to rodents, elicit dramatic increases in the size and number of hepatic and renal peroxisomes, as well as concomitant increases in the capacity of peroxisomes to metabolize fatty acids via increased expression of the enzymes required for the β-oxidation cycle (Lazarow & Fujiki, (1985) *Ann. Rev. Cell Biol.* 1: 489-530; Vamecq & Draye, (1989) *Essays Biochem.* 24: 115-225; and Nelali et al., (1988) *Cancer Res.* 48: 5316-5324). Chemicals of this group include the fibrate class of hypolipidermic drugs, herbicides, phthalate plasticizers, unsaturated fatty acids, and leukotriene antagonists (reviewed in Green, (1992) *Biochem. Pharmacol.* 43: 393-401). Peroxisome proliferation can also be elicited by dietary or physiological factors such as a high-fat diet and cold acclimatization.

Peroxisome proliferator activated receptors (PPARs) are activated by one of a group of compounds known as peroxisome proliferators. Insight into the mechanism by which peroxisome proliferators exert their pleiotropic

effects was provided by the identification of a member of the nuclear hormone receptor superfamily activated by the chemicals described above (Isseman & Green, (1990) *Nature* 347: 645-50). This receptor, termed peroxisome proliferator activated receptor alpha (PPARα), was subsequently shown to be activated by a variety of medium and long-chain fatty acids. PPARα was also shown to modulate expression of a variety of genes containing one or more PPAR responsive elements found in their promoter regions.

It appears that PPARα has a role in the regulation of virtually the entire oxidative pathway of fatty acids and their derivatives (See, Lemberger et al., (1996) *Ann. Rev. Cell. Dev. Biol.* 12: 335-63). It has also been observed that PPARα expression is closely tied to conditions that induce elevated glucocorticoid levels such as fasting, diurnal rhythm (Lemberger et al., (1996) *J. Biol. Chem.* 271: 1764-69) and stress.

Structurally, PPARα comprises three functional domains, the N terminus region, the DNA binding domain and the ligand binding domain. These domains retain their functional autonomy when they are expressed as a chimeric or fusion protein (Göttlicher et al., (1992) *Proc. Natl. Acad. Sci. U.S.A.* 89: 4653-57).

PPARα activates transcription by binding to DNA sequence elements, termed PPAR response elements (PPRE), as heterodimers (dimerization is essential for the activity of PPARs) with the retinoid X receptors (RXR) (See, Keller & Whali, (1993) *Trends Endocrin. Met.* 4: 291-96), which are themselves activated by 9-cis retinoic acid (See, Kliewer et al., (1992) *Nature* 358: 771-74; Gearing et al., (1993) *Proc. Natl. Acad. Sci. U.S.A.* 90: 1440-44; Keller et al., (1993) *Proc. Natl. Acad. Sci. U.S.A.* 90: 2160-2164; Heyman et al., (1992) *Cell* 68: 397-406 and Levin et al., (1992) *Nature* 355: 359-61). Since the PPARα-RXR complex can be activated by peroxisome proliferators and/or 9-cis retinoic acid, the retinoid and fatty acid signaling pathways are seen to converge in modulating lipid metabolism.

PPREs have been identified in the enhancers of a number of genes that encode proteins that regulate lipid metabolism, including: (1) the three

enzymes required for peroxisomal β-oxidation of fatty acids; (2) medium-chain acyl-CoA dehydrogenase, a key enzyme in mitochondrial β-oxidation; and (3) aP2, a lipid binding protein expressed exclusively in adipocytes. Thus, the nature of the PPAR target genes coupled with the activation of PPARs by fatty acids and hypolipidemic drugs suggests a physiological role for the PPARs in a variety of physiological phenomena, including lipid homeostasis (See, e.g., Keller & Whali, (1993) *Trends Endocrin. Met.* 4: 291-96). PPARs have also been implicated in glucose homeostasis disorders and in atherosclerosis. These conditions may exist alone or together in a complex phenotype of metabolic disorders known as syndrome X.

Since the discovery of PPARα, additional subtypes of PPAR have been identified, e.g. PPARγ and PPARδ, which are spatially differentially expressed. Because there are several subtypes of PPAR, it is desirable to identify compounds that are capable of selectively interacting with only one of the PPAR subtypes, notably PPARα. Compounds capable of interacting with PPARα exclusively would find a wide variety of applications, for example, in the prevention of obesity, for the treatment of diabetes, and other deleterious conditions, as noted above. Development of such compounds, however, has been hindered by a lack of detailed structural information on the ligand binding domain of PPARα and particularly by a lack of structural information on the conformation of the ligand binding domain of PPARα as it binds a modulating compound.

It is believed that PPARα regulates some of the same genes as PPARγ and PPARδ. However, some genes might be upregulated by one PPAR and downregulated by another PPAR. Up- or down-regulation of certain genes by a PPARγ agonist might cause detrimental side effects. It might be possible to use a PPARα or PPARδ agonist, partial agonist or antagonist to down- or up-regulate (respectively) these same genes, and thereby reduce the detrimental side-effects. More generally, it might be possible to individually up- and down-regulate specific genes to achieve a specific therapeutic goal by administering a PPAR activator (or partial activator) that activates (or

deactivates) each PPAR to the appropriate extent. Design or discovery of such a compound would be greatly facilitated by three-dimensional structures for each of the three target receptors, PPARα, PPARγ and PPARδ.

Polypeptides, including the ligand binding domain of PPARα, have a three-dimensional structure determined by the primary amino acid sequence and the environment surrounding the polypeptide. This three-dimensional structure establishes the polypeptide's activity, stability, binding affinity, binding specificity, and other biochemical attributes. Thus, knowledge of a protein's three-dimensional structure can provide much guidance in designing agents that mimic, inhibit, or improve its biological activity.

The three-dimensional structure of a polypeptide can be determined in a number of ways. Many of the most precise methods employ X-ray crystallography (See, e.g., Van Holde, (1971) Physical Biochemistry, Prentice-Hall, N. J., 221-39). This technique relies on the ability of crystalline lattices to diffract X-rays or other forms of radiation. Diffraction experiments suitable for determining the three-dimensional structure of macromolecules typically require high-quality crystals. Unfortunately, such crystals have been unavailable for the ligand binding domain of PPARα, as well as many other proteins of interest. Thus, high-quality diffracting crystals of the ligand binding domain of PPARα in complex with a ligand would greatly assist in the elucidation of its three-dimensional structure.

Clearly, the solved crystal structure of the PPARα ligand binding domain polypeptide would be useful in the design of modulators of activity mediated by all of the PPARs. Evaluation of the available sequence data has made it clear that PPARα shares significant sequence homology with the other PPARs. Further, PPARα shows structural homology with the three-dimensional fold of the other PPARs. Thus, in theory, it might be considered feasible to design modulators of PPARα based exclusively on the sequence and three-dimensional fold of a different PPAR, for example, PPARγ. This method, however, would likely be unproductive and certainly hindered by a lack of subtle structural details of the various binding sites and pertinent

residues of PPARα involved in the binding event. A solved crystal structure would provide these structural details.

The solved PPARα-ligand crystal structure would provide structural details and insights necessary to design a modulator of PPARα that maximizes preferred requirements for any modulator, i.e. potency and specificity. By exploiting the structural details obtained from a PPAR-ligand crystal structure, it would be possible to design a PPAR modulator that, despite PPARα's similarity with other PPARs, exploits the unique structural features of PPARα. A PPAR modulator developed using structure-assisted design would take advantage of heretofore unknown PPAR structural considerations and thus be more effective than a modulator developed using homology-based design. Potential or existent homology models cannot provide the necessary degree of specificity. A PPAR modulator designed using the structural coordinates of a crystalline form of PPARα would also provide a starting point for the development of modulators of other PPARs.

What is needed, therefore, is a crystallized form of a PPARα ligand binding domain, preferably in complex with a ligand. Acquisition of crystals of the PPARα ligand binding domain (LBD) polypeptide will permit the three dimensional structure of PPARα LBD polypeptide to be determined. Knowledge of the three dimensional structure will facilitate the design of modulators of PPARα activity. Such modulators can lead to therapeutic compounds to treat a wide range of conditions, including lipid homeostasis disorders, glucose homeostasis disorders, inflammation, atherosclerosis and syndrome X.

Summary of the Invention

A substantially pure PPARα ligand binding domain polypeptide in crystalline form is disclosed. Preferably, the crystalline form has lattice constants of a = 61.3 Å, b = 103.5 Å, c = 49.9 Å, α = 90°, β = 90°, γ = 90° or lattice constants of a = 95.58 Å, b = 122.06 Å, c = 122.10 Å, α = 90°, β = 90°, γ = 90°. Preferably, the crystalline form is an orthorhombic crystalline form.

More preferably, the crystalline form has a space group of $P2_12_12$ or space group $P2_12_12_1$. Even more preferably, the PPARα ligand binding domain polypeptide has the amino acid sequence shown in SEQ ID NO: 4. Even more preferably, the PPARα ligand binding domain has a crystalline structure further characterized by the coordinates corresponding to Table 2.

Preferably, the PPARα ligand binding domain polypeptide is in complex with a ligand. Optionally, the crystalline form contains one or four PPARα ligand binding domain polypeptides in the asymmetric unit. Preferably, the crystalline form is such that the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide can be determined to a resolution of about 1.8 Å or better. Even more preferably, the crystalline form contains one or more atoms having a molecular weight of 40 grams/mol or greater.

A method for determining the three-dimensional structure of a crystallized PPARα ligand binding domain polypeptide to a resolution of about 1.8 Å or better is disclosed. The method comprises (a) crystallizing a PPARα ligand binding domain polypeptide; and (b) analyzing the PPARα ligand binding domain polypeptide to determine the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide, whereby the three-dimensional structure of a crystallized PPARα ligand binding domain polypeptide is determined to a resolution of about 1.8 Å or better. Preferably, the analyzing is by X-ray diffraction. More preferably, the crystallization is accomplished by the hanging drop vapor diffusion method, and wherein the PPARα ligand binding domain is mixed with an equal volume of reservoir. Even more preferably, the reservoir comprises 4-8% PEG 3350, 100-200mM NaF, and 12-16% 2,5 hexanediol or the reservoir comprises 50 mM bis-tris-propane, 4-6% PEG 3350, 150 mM $NaNO_3$, 16% 2,5 hexanediol, and 1-3 mM YCl_3.

A method of designing a modulator of a PPAR polypeptide is disclosed. The method comprises (a) designing a potential modulator of a PPAR polypeptide that will form bonds with amino acids in a substrate binding site based upon a crystalline structure of a PPARα ligand binding domain

polypeptide; (b) synthesizing the modulator; and (c) determining whether the potential modulator modulates the activity of the PPAR polypeptide, whereby a modulator of a PPAR polypeptide is designed.

A method of designing a modulator that selectively modulates the activity of a PPAR polypeptide is disclosed. The method comprises (a) obtaining a crystalline form of a PPARα ligand binding domain polypeptide; (b) evaluating the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide; and (c) synthesizing a potential modulator based on the three-dimensional crystal structure of the crystallized PPARα ligand binding domain polypeptide, whereby a modulator that selectively modulates the activity of a PPARα polypeptide is designed. Preferably, the method further comprises contacting a PPARα ligand binding domain polypeptide with the potential modulator; and assaying the PPARα ligand binding domain polypeptide for binding of the potential modulator, for a change in activity of the PPARα ligand binding domain polypeptide, or both. More preferably, the crystalline form is in orthorhombic form. Even more preferably, the crystals are such that the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide can be determined to a resolution of about 1.8 Å or better.

A method of screening a plurality of compounds for a modulator of a PPAR ligand binding domain polypeptide is disclosed. The method comprises (a) providing a library of test samples; (b) contacting a crystalline PPARα ligand binding domain polypeptide with each test sample; (c) detecting an interaction between a test sample and the crystalline PPARα ligand binding domain polypeptide; (d) identifying a test sample that interacts with the crystalline PPARα ligand binding domain polypeptide; and (e) isolating a test sample that interacts with the crystalline PPARα ligand binding domain polypeptide, whereby a plurality of compounds is screened for a modulator of a PPAR ligand binding domain polypeptide. Preferably, the test samples are bound to a substrate, and more preferably, the test samples are synthesized directly on a substrate.

A method for identifying a PPAR modulator is disclosed. The method comprises (a) providing atomic coordinates of a PPARα ligand binding domain to a computerized modeling system; and (b) modeling ligands that fit spatially into the binding pocket of the PPARα ligand binding domain to thereby identify a PPAR modulator. Preferably, the method further comprises identifying in an assay for PPAR-mediated activity a modeled ligand that increases or decreases the activity of the PPAR.

A method of identifying a PPARα modulator that selectively modulates the activity of a PPARα polypeptide compared to other polypeptides is disclosed. The method comprises (a) providing atomic coordinates of a PPARα ligand binding domain to a computerized modeling system; and (b) modeling a ligand that fits into the binding pocket of a PPARα ligand binding domain and that interacts with conformationally constrained residues of a PPARα conserved among PPAR subtypes to thereby identify a PPARα modulator. Preferably, the method further comprises identifying in a biological assay for PPARα activity a modeled ligand that selectively binds to PPARα and increases or decreases the activity of said PPARα.

A method of designing a modulator of a PPAR polypeptide is disclosed. The method comprises (a) selecting a candidate PPAR ligand; (b) determining which amino acid or amino acids of a PPAR polypeptide interact with the ligand using a three-dimensional model of a crystallized protein comprising a PPARα LBD; (c) identifying in a biological assay for PPAR activity a degree to which the ligand modulates the activity of the PPAR polypeptide; (d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the PPAR polypeptide and the ligand is predicted to be modulated by the chemical modification; (e) performing the chemical modification on the ligand to form a modified ligand; (f) contacting the modified ligand with the PPAR polypeptide; (g) identifying in a biological assay for PPAR activity a degree to which the modified ligand modulates the biological activity of the PPAR polypeptide; and (h) comparing the biological activity of the PPAR polypeptide in the presence of modified ligand with the

biological activity of the PPAR polypeptide in the presence of the unmodified ligand, whereby a modulator of a PPAR polypeptide is designed. Preferably, the PPAR polypeptide is a PPARα polypeptide. More preferably, the three-dimensional model of a crystallized protein is a PPARα LBD polypeptide with a bound ligand. Optionally, the method further comprises repeating steps (a) through (f), if the biological activity of the PPAR polypeptide in the presence of the modified ligand varies from the biological activity of the PPAR polypeptide in the presence of the unmodified ligand.

An assay method for identifying a compound that inhibits binding of a ligand to a PPAR polypeptide is disclosed. The assay method comprises (a) incubating a PPAR polypeptide with a ligand in the presence of a test inhibitor compound; (b) determining an amount of ligand that is bound to the PPAR polypeptide; wherein decreased binding of ligand to the PPAR protein in the presence of the test inhibitor compound relative to binding of ligand in the absence of the test inhibitor compound is indicative of inhibition; and (c) identifying the test compound as an inhibitor of ligand binding if decreased ligand binding is observed.

A method of identifying a PPAR modulator that selectively modulates the biological activity of one PPAR subtype compared to PPARα is disclosed. The method comprises: (a) providing an atomic structure coordinate set describing a PPARα ligand binding domain structure and at least one other atomic structure coordinate set describing a PPAR ligand binding domain, each ligand binding domain comprising a ligand binding site; (b) comparing the PPAR atomic structure coordinate sets to identify at least one diference between the sets; (c) designing a candidate ligand predicted to interact with the difference of step (b); (d) synthesizing the candidate ligand; and (e) testing the synthesized candidate ligand for an ability to selectively modulate a PPAR subtype as compared to PPARα, whereby a PPAR modulator that selectively modulates the biological activity of one PPAR subtype compared to PPARα is identified.

Accordingly, it is an object of the present invention to provide a three dimensional structure of the ligand binding domain of PPARα. The object is

achieved in whole or in part by the present invention.

An object of the invention having been stated hereinabove, other objects will be evident as the description proceeds, when taken in connection with the accompanying Drawings and Laboratory Examples as best described hereinbelow.

Brief Description of the Drawings

Figure 1 is a ribbon diagram depicting the PPARα LBD in complex with Compound 1. The PPARα LBD is presented as a ribbon diagram and Compound 1 is presented as a spacefilling model.

Figure 2 is a schematic drawing depicting interactions between PPARα and Compound 1. Residues that lie within 5.5Å of heavy atoms in the ligand are shown.

Figure 3 depicts overlayed ball and stick diagrams of PPARα, PPARγ and PPARδ. PPARα is shown in dark gray, PPARγ in medium gray and PPARδ in light gray. PPARδ was used as a template in the molecular replacement solution of PPARα.

Figure 4 is a ribbon diagram of the PPARα backbone conformation, where the ligand binding pocket of PPARα is identified by a smooth solid surface.

Figure 5 is a ribbon diagram of the PPARγ backbone conformation, where the ligand binding pocket of PPARγ is identified by a smooth solid surface.

Figure 6 is a ribbon diagram of the PPARδ backbone conformation, where the ligand binding pocket of PPARδ is identified by a smooth solid surface.

Figure 7 is a ball-and-stick model depicting hydrogen bonding interactions between Compound 1 and PPARα. Water molecules are shown as octahedral (six-pointed) crosses.

Detailed Description of the Invention

Until disclosure of the present invention presented herein, the ability to obtain crystalline forms of a PPARα LBD has not been realized. And until disclosure of the present invention presented herein, a detailed three-dimensional crystal structure of a PPARα polypeptide has not been solved.

In addition to providing structural information, crystalline polypeptides provide other advantages. For example, the crystallization process itself further purifies the polypeptide, and satisfies one of the classical criteria for homogeneity. In fact, crystallization frequently provides unparalleled purification quality, removing impurities that are not removed by other purification methods such as HPLC, dialysis, conventional column chromatography, etc. Moreover, crystalline polypeptides are often stable at ambient temperatures and free of protease contamination and other degradation associated with solution storage. Crystalline polypeptides can also be useful as pharmaceutical preparations. Finally, crystallization techniques in general are largely free of problems such as denaturation associated with other stabilization methods (e.g., lyophilization). Once crystallization has been accomplished, crystallographic data provides useful structural information that can assist the design of compounds that can serve as agonists or antagonists, as described herein below. In addition, the crystal structure provides information useful to map a receptor binding domain, which could then be mimicked by a small non-peptide molecule that would serve as an antagonist or agonist.

I. Definitions

Following long-standing patent law convention, the terms "a" and "an" mean "one or more" when used in this application, including the claims.

As used herein, the term "mutation" carries its traditional connotation and means a change, inherited, naturally occurring or introduced, in a nucleic acid or polypeptide sequence, and is used in its sense as generally known to those of skill in the art.

As used herein, the term "labeled" means the attachment of a moiety, capable of detection by spectroscopic, radiologic or other methods, to a probe molecule.

As used herein, the term "target cell" refers to a cell, into which it is desired to insert a nucleic acid sequence or polypeptide, or to otherwise effect a modification from conditions known to be standard in the unmodified cell. A nucleic acid sequence introduced into a target cell can be of variable length. Additionally, a nucleic acid sequence can enter a target cell as a component of a plasmid or other vector or as a naked sequence.

As used herein, the term "transcription" means a cellular process involving the interaction of an RNA polymerase with a gene that directs the expression as RNA of the structural information present in the coding sequences of the gene. The process includes, but is not limited to the following steps: (a) the transcription initiation, (b) transcript elongation, (c) transcript splicing, (d) transcript capping, (e) transcript termination, (f) transcript polyadenylation, (g) nuclear export of the transcript, (h) transcript editing, and (i) stabilizing the transcript.

As used herein, the term "expression" generally refers to the cellular processes by which a biologically active polypeptide is produced.

As used herein, the term "transcription factor" means a cytoplasmic or nuclear protein which binds to such gene, or binds to an RNA transcript of such gene, or binds to another protein which binds to such gene or such RNA transcript or another protein which in turn binds to such gene or such RNA transcript, so as to thereby modulate expression of the gene. Such modulation can additionally be achieved by other mechanisms; the essence of "transcription factor for a gene" is that the level of transcription of the gene is altered in some way.

As used herein, the term "hybridization" means the binding of a probe molecule, a molecule to which a detectable moiety has been bound, to a target sample.

As used herein, the term "detecting" means confirming the presence of a target entity by observing the occurrence of a detectable signal, such as a

radiologic or spectroscopic signal that will appear exclusively in the presence of the target entity.

As used herein, the term "sequencing" means the determining the ordered linear sequence of nucleic acids or amino acids of a DNA or protein target sample, using conventional manual or automated laboratory techniques.

As used herein, the term "isolated" means oligonucleotides substantially free of other nucleic acids, proteins, lipids, carbohydrates or other materials with which they can be associated, such association being either in cellular material or in a synthesis medium. The term can also be applied to polypeptides, in which case the polypeptide will be substantially free of nucleic acids, carbohydrates, lipids and other undesired polypeptides.

As used herein, the term "substantially pure" means that the polynucleotide or polypeptide is substantially free of the sequences and molecules with which it is associated in its natural state, and those molecules used in the isolation procedure. The term "substantially free" means that the sample is at least 50%, preferably at least 70%, more preferably 80% and most preferably 90% free of the materials and compounds with which is it associated in nature.

As used herein, the term "primer" means a sequence comprising two or more deoxyribonucleotides or ribonucleotides, preferably more than three, and more preferably more than eight and most preferably at least about 20 nucleotides of an exonic or intronic region. Such oligonucleotides are preferably between ten and thirty bases in length.

As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences. Preferred embodiments of genomic and cDNA sequences are disclosed herein.

As used herein, the term "DNA segment" means a DNA molecule that has been isolated free of total genomic DNA of a particular species. In a preferred embodiment, a DNA segment encoding a PPARα polypeptide refers

to a DNA segment that comprises SEQ ID NOs: 1 and 3, but can optionally comprise fewer or additional nucleic acids, yet is isolated away from, or purified free from, total genomic DNA of a source species, such as *Homo sapiens*. Included within the term "DNA segment" are DNA segments and smaller fragments of such segments, and also recombinant vectors, including, for example, plasmids, cosmids, phages, viruses, and the like.

As used herein, the phrase "enhancer-promoter" means a composite unit that contains both enhancer and promoter elements. An enhancer-promoter is operatively linked to a coding sequence that encodes at least one gene product.

As used herein, the phrase "operatively linked" means that an enhancer-promoter is connected to a coding sequence in such a way that the transcription of that coding sequence is controlled and regulated by that enhancer-promoter. Techniques for operatively linking an enhancer-promoter to a coding sequence are well known in the art; the precise orientation and location relative to a coding sequence of interest is dependent, *inter alia*, upon the specific nature of the enhancer-promoter.

As used herein, the terms "candidate substance" and "candidate compound" are used interchangeably and refer to a substance that is believed to interact with another moiety, for example a given ligand that is believed to interact with a complete, or a fragment of, a PPAR polypeptide, and which can be subsequently evaluated for such an interaction. Representative candidate substances or compounds include xenobiotics such as drugs and other therapeutic agents, carcinogens and environmental pollutants, natural products and extracts, as well as endobiotics such as steroids, fatty acids and prostaglandins. Other examples of candidate compounds that can be investigated using the methods of the present invention include, but are not restricted to, agonists and antagonists of a PPAR polypeptide, toxins and venoms, viral epitopes, hormones (e.g., opioid peptides, steroids, etc.), hormone receptors, peptides, enzymes, enzyme substrates, co-factors, lectins, sugars, oligonucleotides or nucleic acids, oligosaccharides, proteins, small molecules and monoclonal antibodies.

As used herein, the term "biological activity" means any observable effect flowing from interaction between a PPAR polypeptide and a ligand. Representative, but non-limiting, examples of biological activity in the context of the present invention include dimerization of PPARα with RXR, phosphorylation, and association of PPARα with DNA.

As used herein, the term "modified" means an alteration from an entity's normally occurring state. An entity can be modified by removing discrete chemical units or by adding discrete chemical units. The term "modified" encompasses detectable labels as well as those entities added as aids in purification.

As used herein, the terms "structure coordinates" and "structural coordinates" mean mathematical coordinates derived from mathematical equations related to the patterns obtained on diffraction of a monochromatic beam of X-rays by the atoms (scattering centers) of a molecule in crystal form. The diffraction data are used to calculate an electron density map of the repeating unit of the crystal. The electron density maps are used to establish the positions of the individual atoms within the unit cell of the crystal.

Those of skill in the art understand that a set of structure coordinates determined by X-ray crystallography is not without standard error. For the purpose of this invention, any set of structure coordinates for PPARα or a PPARα mutant that have a root mean square (RMS) deviation of no more than 1.0 Å when superimposed, using the polypeptide backbone atoms, on the structure coordinates listed in Table 2 shall be considered identical.

As used herein, the term "space group" means the arrangement of symmetry elements of a crystal.

As used herein, the term "molecular replacement" means a method that involves generating a preliminary model of the wild-type PPARα ligand binding domain, or a PPARα mutant crystal whose structure coordinates are unknown, by orienting and positioning a molecule whose structure coordinates are known (e.g., PPARδ) within the unit cell of the unknown crystal so as best to account for the observed diffraction pattern of the unknown crystal. Phases can then be calculated from this model and

combined with the observed amplitudes to give an approximate Fourier synthesis of the structure whose coordinates are unknown. This, in turn, can be subject to any of the several forms of refinement to provide a final, accurate structure of the unknown crystal. (Lattman, (1985) *Method Enzymol.*, 115: 55-77; Rossmann, ed, (1972) The Molecular Replacement Method, Gordon & Breach, New York.) Using the structure coordinates of the ligand binding domain of PPARα provided by this invention, molecular replacement can be used to determine the structure coordinates of a crystalline mutant or homologue of the PPARα ligand binding domain, or of a different crystal form of the PPARα ligand binding domain.

As used herein, the terms "β-sheet" and "beta-sheet" mean the conformation of a polypeptide chain stretched into an extended zig-zig conformation. Portions of polypeptide chains that run "parallel" all run in the same direction. Polypeptide chains that are "antiparallel" run in the opposite direction from the parallel chains.

As used herein, the terms "α-helix" and "alpha-helix" mean the conformation of a polypeptide chain wherein the polypeptide backbone is wound around the long axis of the molecule in a left-handed or right-handed direction, and the R groups of the amino acids protrude outward from the helical backbone, wherein the repeating unit of the structure is a single turnoff the helix, which extends about 0.56 nm along the long axis.

As used herein, the term "unit cell" means a basic parallelipiped shaped block. The entire volume of a crystal can be constructed by regular assembly of such blocks. Each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal. Thus, the term "unit cell" means the fundamental portion of a crystal structure that is repeated infinitely by translation in three dimensions. A unit cell is characterized by three vectors a, b, and c, not located in one plane, which form the edges of a parallelepiped. Angles α, β and γ define the angles between the vectors: angle α is the angle between vectors b and c; angle β is the angle between vectors a and c; and angle γ is the angle between vectors

a and b. The entire volume of a crystal can be constructed by regular assembly of unit cells; each unit cell comprises a complete representation of the unit of pattern, the repetition of which builds up the crystal.

As used herein, "orthorhombic unit cell" means a unit cell wherein $a \neq b \neq c$; and $\alpha = \beta = \gamma = 90°$. The vectors a, b and c describe the unit cell edges and the angles α, β, and γ describe the unit cell angles.

As used herein, the term "crystal lattice" means the array of points defined by the vertices of packed unit cells.

As used herein, the term "PPAR" means any polypeptide sequence that can be aligned with at least one of human PPARα, PPARγ or PPARδ such that at least 50% of the amino acids are identical to the corresponding amino acid in the human PPARα, PPARγ or PPARδ. The term "PPAR" also encompasses nucleic acid sequences where the corresponding translated protein sequence can be considered to be a PPAR. The term "PPAR" encompasses at least the PPARα, PPARγ and PPARδ subtypes. The term "PPAR" includes invertebrate homologs; preferably, PPAR nucleic acids and polypeptides are isolated from eukaryotic sources. "PPAR" further includes vertebrate homologs of PPAR family members, including, but not limited to, mammalian and avian homolog. Representative mammalian homologs of PPAR family members include, but are not limited to, murine and human homologs.

As used herein, the terms "PPARα gene product", "PPARα protein", "PPARα polypeptide", and "PPARα peptide" are used interchangeably and mean peptides having amino acid sequences which are substantially identical to native amino acid sequences from the organism of interest and which are biologically active in that they comprise all or a part of the amino acid sequence of a PPARα polypeptide, or cross-react with antibodies raised against a PPARα polypeptide, or retain all or some of the biological activity (e.g., DNA or ligand binding ability and/or dimerization ability) of the native amino acid sequence or protein. Such biological activity can include immunogenicity.

In the present invention, the terms "PPARα gene product", "PPARα protein", "PPARα polypeptide", and "PPARα peptide" are used interchangeably and mean to the preferred subtype of the PPAR family, namely PPARα, which comprises the amino acid sequence of SEQ ID NO: 2.

As used herein, the terms "PPARα gene product", "PPARα protein", "PPARα polypeptide", and "PPARα peptide" also include analogs of a PPARα polypeptide. By "analog@ is intended that a DNA or peptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences as are disclosed herein or from other organisms, or can be created synthetically. Those skilled in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct PPARα analogs. There is no need for a "PPARα gene product", "PPARα protein", "PPARα polypeptide", or "PPARα peptide" to comprise all or substantially all of the amino acid sequence of a PPARα polypeptide gene product. Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "PPARα gene product", "PPARα protein", "PPARα polypeptide", and "PPARα peptide" also include fusion or recombinant PPARα polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein and are known in the art.

As used herein, the term "polypeptide" means any polymer comprising any of the 20 protein amino acids, regardless of its size. Although "protein" is often used in reference to relatively large polypeptides, and "peptide" is often used in reference to small polypeptides, usage of these terms in the art overlaps and varies. The term "polypeptide" as used herein refers to peptides, polypeptides and proteins, unless otherwise noted. As used herein, the terms "protein", "polypeptide" and "peptide" are used interchangeably herein when referring to a gene product.

As used herein, the term "modulate" means an increase, decrease, or other alteration of any or all chemical and biological activities or properties of a wild-type or mutant PPAR polypeptide, preferably a wild-type or mutant PPARα polypeptide. The term "modulation" as used herein refers to both upregulation (i.e., activation or stimulation) and downregulation (i.e. inhibition or suppression) of a response.

As used herein, the terms "binding pocket of the PPARα ligand binding domain", "PPARα ligand binding pocket" and "PPARα binding pocket" are used interchangeably, and refer to the large cavity within the PPARα ligand binding domain where Compound 1 binds. This cavity may be empty, or may contain water molecules or other molecules from the solvent, or may contain ligand atoms. The "main" binding pocket includes the region of space not occupied by atoms of PPARα that comprises residues Ile-241, Leu-247, Ala-250, Glu-251, Leu-254, Val-255, Ile-272, Phe-273, Cys-275, Cys-276, Gln-277, Thr-279, Ser-280, Tyr-314, Ile-317, Phe-318, Leu-321, Met-330, Val-332, Ala-333, Ile-339, Leu-344, Ile-354, Met-355, His- 440, Val-444, Leu-456, Leu-460 and Tyr-464. The binding pocket also includes regions of space near the "main" binding pocket that not occupied by atoms of PPARα but that are near the "main" binding pocket, and that are contiguous with the "main" binding pocket.

As used herein, the terms "PPAR gene" and "recombinant PPAR gene" mean a nucleic acid molecule comprising an open reading frame encoding a PPAR polypeptide of the present invention, including both exon and (optionally) intron sequences.

As used herein, the term "gene" is used for simplicity to refer to a functional protein, polypeptide or peptide encoding unit. As will be understood by those in the art, this functional term includes both genomic sequences and cDNA sequences. Preferred embodiments of genomic and cDNA sequences are disclosed herein.

As used herein, the term "DNA sequence encoding a PPAR polypeptide" can refer to one or more coding sequences within a particular individual. Moreover, certain differences in nucleotide sequences can exist

between individual organisms, which are called alleles. It is possible that such allelic differences might or might not result in differences in amino acid sequence of the encoded polypeptide yet still encode a protein with the same biological activity. As is well known, genes for a particular polypeptide can exist in single or multiple copies within the genome of an individual. Such duplicate genes can be identical or can have certain modifications, including nucleotide substitutions, additions or deletions, all of which still code for polypeptides having substantially the same activity.

As used herein, the term "intron" means a DNA sequence present in a given gene that is not translated into protein.

As used herein, the term "interact" means detectable interactions between molecules, such as can be detected using, for example, a yeast two hybrid assay. The term "interact" is also meant to include "binding" interactions between molecules. Interactions can, for example, be protein-protein or protein-nucleic acid in nature.

As used herein, the terms "cells," "host cells" or "recombinant host cells" are used interchangeably and mean not only to the particular subject cell, but also to the progeny or potential progeny of such a cell. Because certain modifications can occur in succeeding generations due to either mutation or environmental influences, such progeny might not, in fact, be identical to the parent cell, but are still included within the scope of the term as used herein.

As used herein, the term "agonist" means an agent that supplements or potentiates the bioactivity of a functional PPAR gene or protein or of a polypeptide encoded by a gene that is up- or down-regulated by a PPAR polypeptide and/or a polypeptide encoded by a gene that contains a PPAR binding site or response element in its promoter region.

As used herein, the term "antagonist" means an agent that decreases or inhibits the bioactivity of a functional PPAR gene or protein, or that supplements or potentiates the bioactivity of a naturally occurring or engineered non-functional PPAR gene or protein. Alternatively, an antagonist can decrease or inhibit the bioactivity of a functional gene or polypeptide

encoded by a gene that is up- or down-regulated by a PPAR polypeptide and/or contains a PPAR binding site or response element in its promoter region. An antagonist can also supplement or potentiate the bioactivity of a naturally occurring or engineered non-functional gene or polypeptide encoded by a gene that is up- or down-regulated by a PPAR polypeptide, and/or contains a PPAR binding site or response element in its promoter region.

As used herein, the terms "chimeric protein" or "fusion protein" are used interchangeably and mean a fusion of a first amino acid sequence encoding a PPAR polypeptide with a second amino acid sequence defining a polypeptide domain foreign to, and not homologous with, any domain of a PPAR polypeptide. A chimeric protein can include a foreign domain that is found in an organism that also expresses the first protein, or it can be an "interspecies" or "intergenic" fusion of protein structures expressed by different kinds of organisms. In general, a fusion protein can be represented by the general formula X—PPAR—Y, wherein PPAR represents a portion of the protein which is derived from a PPAR polypeptide, and X and Y are independently absent or represent amino acid sequences which are not related to a PPAR sequence in an organism, which includes naturally occurring mutants.

II. Description of Tables

Table 1 is a table summarizing the crystal and data statistics obtained from the crystallized ligand binding domain of PPARα. Data on the unit cell are presented, including data on the crystal space group, unit cell dimensions, molecules per asymmetric cell and crystal resolution.

Table 2 is a table of the atomic structure coordinate data obtained from X-ray diffraction from the ligand binding domain of PPARα in complex with a ligand.

Table 3 is a table of the atomic structure coordinate data obtained from X-ray diffraction from the ligand binding domain (residues 207-441) of a PPARδ crystal (Xu et al., (1999) *Mol. Cell* 3: 397-403, PDB ID: 1GWX; Genbank Accession No. L07592; available online at http://www.rcsb.org/pdb/).

The coordinate data from the PPARδ ligand binding domain were used in the molecular replacement solution of the PPARα ligand binding domain crystal form.

Table 4 is a sequence alignment which shows sequence similarities between the PPARα, PPARγ and PPARδ sequences. The binding site residues are denoted by small boxes and represent those residues lying within 5.0 angstroms of the ligand.

III. General Considerations

The present invention will usually be applicable *mutatis mutandis* to all PPARs, as discussed herein based, in part, on the patterns of PPAR structure and modulation that have emerged as a consequence of determining the three dimensional structure of PPARα with bound ligand. Analysis and alignment of amino acid sequences, and X-ray and NMR structure determinations, have shown that nuclear receptors have a modular architecture with three main domains:

1) a variable amino-terminal domain;

2) a highly conserved DNA-binding domain (DBD); and

3) a less conserved carboxy-terminal ligand binding domain (LBD).

In addition, nuclear receptors may have linker segments of variable length between these major domains. Sequence analysis and X-ray crystallography, including the work of the present invention, have confirmed that PPARs also have the same general modular architecture, with the same three domains. The function of the PPARs in human cells presumably requires all three domains in a single amino acid sequence. However, the modularity of the PPARs permits different domains of each protein to separately accomplish certain functions. Some of the functions of a domain within the full-length receptor are preserved when that particular domain is isolated from the remainder of the protein. Using conventional protein chemistry techniques, a modular domain can sometimes be separated from the parent protein. Using conventional molecular biology techniques, each domain can usually be separately expressed with its original function intact or, as discussed herein

below, chimeras comprising two different proteins can be constructed, wherein the chimeras retain the properties of the individual functional domains of the respective nuclear receptors from which the chimeras were generated.

The amino terminal domain of the PPAR subtypes is the least conserved of the three domains. This domain is involved in transcriptional activation and, in some cases, its uniqueness may dictate selective receptor-DNA binding and activation of target genes by PPAR subtypes. This domain can display synergistic and antagonistic interactions with the domains of the LBD.

The DNA binding domain has the most highly conserved amino acid sequence amongst the PPARs. It typically contains about 70 amino acids that fold into two zinc finger motifs, wherein a zinc atom coordinates four cysteines. The DBD contains two perpendicularly oriented α-helixes that extend from the base of the first and second zinc fingers. The two zinc fingers function in concert along with non-zinc finger residues to direct the PPAR to specific target sites on DNA and to align receptor heterodimer interfaces. Various amino acids in the DBD influence spacing between two half-sites (which usually comprises six nucleotides) for receptor heterodimerization. The optimal spacings facilitate cooperative interactions between DBDs, and D box residues are part of the dimerization interface. Other regions of the DBD facilitate DNA-protein and protein-protein interactions required for RXR-PPAR heterodimerization.

The LBD is the second most highly conserved domain in these receptors. As its name suggest, the LBD binds ligands. With many nuclear receptors, including the PPARs, binding of the ligand can induce a conformational change in the LBD that can, in turn, activate transcription of certain target genes. The LBD also participates in other functions, including dimerization and nuclear translocation.

X-ray structures have shown that most nuclear receptor LBDs adopt the same general folding pattern. This fold consists of 10-12 alpha-helices arranged in a bundle, together with several beta-strands, additional alpha-helices and linking segments. The major alpha helices and beta-strands

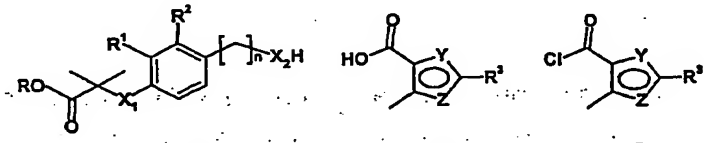
have been numbered differently in different publications. This patent will follow the numbering scheme of Nolte et al., (Nolte et al., (1998) *Nature* 395:137-43), where the major alpha-helices and beta-strands are designated sequentially through the amino acid sequence as H1, H2, S1, H2', H3, H3', H4, H5, S2, S3, S4, H6, H7, H8, H9, H10 and HAF. The alpha-helix at the C-terminal end, HAF, is also called "helix-AF", "helix-AF2" or the "AF2 helix". Structural studies have shown that most of the alpha-helices and beta-strands have the same general position and orientation in all nuclear receptor structures, whether ligand is bound or not. However, the AF2 helix has been found in different positions and orientations relative to the main bundle, depending on the presence or absence of the ligand, and also on the chemical nature of the ligand. These structural studies have suggested that many nuclear receptors share a common mechanism of activation, where binding of activating ligands helps to stabilize the AF2 helix in a position and orientation adjacent to helices-3, -4, and –10, covering an opening to the ligand binding site. This position and orientation of the AF2 helix, which will be called the "active conformation", creates a binding site for coactivators. See, e.g., Nolte et al., (1998) *Nature* 395:137-43; Shiau et al., (1998) *Cell* 95: 927-37. This coactivator binding site has a central lipophilic pocket that can accommodate leucine side-chains from coactivators, as well as a "charge-clamp" structure consisting primarily of a lysine residue from helix-3 and a glutamic acid residue from the AF2 helix. Structural studies have shown that coactivator peptides containing the sequence LXXLL (where L is leucine and X can be a different amino acid in different cases) can bind to this coactivator binding site by making interactions with the charge clamp lysine and glutamic acid residues, as well as the central lipophilic region. This coactivator binding site is disrupted when the AF2 helix is shifted into other positions and orientations. In PPAR-γ, activating ligands such as rosiglitazone (BRL49653) make a hydrogen bonding interaction with tyrosine-473 in the AF2 helix. Nolte et al., (1998) *Nature* 395:137-43; Gampe et al., (2000) *Mol. Cell* 5: 545-55. This interaction is believed to stabilize the AF2 helix in the active conformation, thereby allowing coactivators to bind and thus activating

transcription from target genes. With certain antagonist ligands, or in the absence of any ligand, the AF2 helix may be held less tightly in the active conformation, or may be free to adopt other conformations. This would either destabilize or disrupt the coactivator binding site, thereby reducing or eliminating coactivator binding and transcription from certain target genes. Some of the functions of the PPAR protein depend on having the full-length amino acid sequence and certain partner molecules, such as coactivators and DNA. However, other functions, including ligand binding and ligand-dependent conformational changes, may be observed experimentally using isolated domains, chimeras and mutant molecules.

As described herein, the LBD of a PPAR can be expressed, crystallized, its three dimensional structure determined with a ligand bound as disclosed in the present invention, and computational methods can be used to design ligands to its LBD.

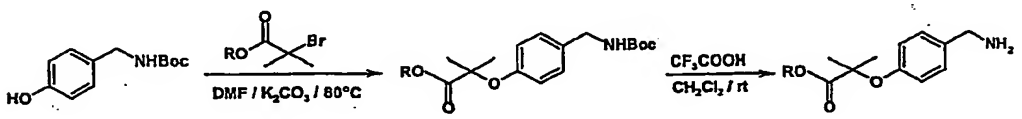
IV. Synthesis of Compound 1 and Intermediates

Compound 1, which was co-crystallized with the PPARα LBD in the present invention, can be conveniently prepared by a general process wherein a moiety like **(A)** is coupled to an acid **(B)** using a peptide coupling reaction or by alkylation of **(A)** using a suitable non nucleophilic amine with an acid chloride **(C)**. Preferably, R is 1-6 alkyl, which can be hydrolyzed off or, is readily hydrolyzable.



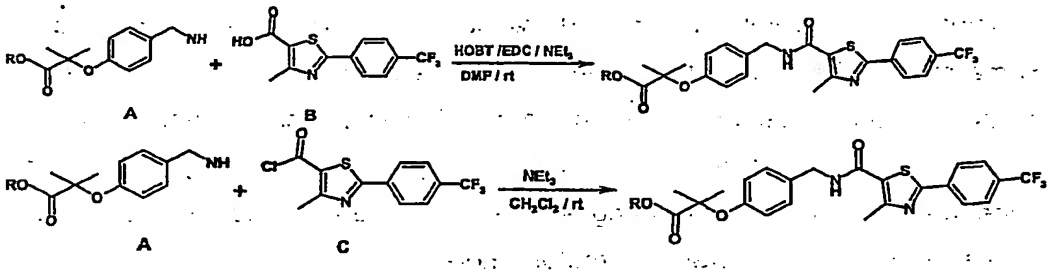
A B C

A preferred synthesis of **(A)** when X_1 is O and X_2 is NH (and R^1 and R^2 are H) is:



A

Note that this synthesis is preferably carried out with the amine where the alcohol function is already alkylated with the acid side chain protected by R.. For example, when n is1, X_1 is O, X_2 is NH, Y is S, Z is N, R^1 and R^2 are H, and R^3 is 4-F_3C-phenyl :

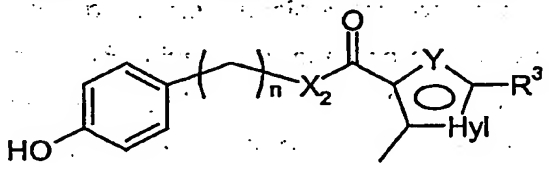


A B

A C

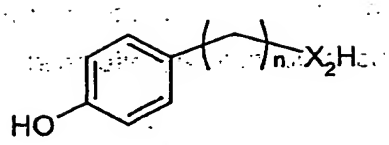
Some of the intermediates of type **A** are commercially available while others can be synthesized by techniques apparent to a person skilled in the art. The synthesis of intermediates of type **B** is illustrated below.

Compound 1 can be made by an alternative method in which compounds of formula **(D)** are reacted with ethyl 2-bromo-2 methyl propionate to produce an ethyl ester, which may be hydrolyzed to produce the free acid.



D

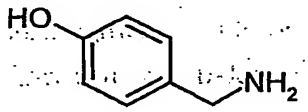
Compounds of formula **(D)** may be prepared from the reaction between compounds of formula **(B)** and compounds of formula **(E)** with HOBT / EDC / NEt_3 when X_2 is NH or NCH_3 or DIC / DMAP / NEt_3 when X_2 is O.



E

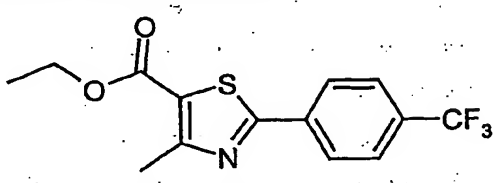
The invention is further illustrated by the following examples which should not be construed as constituting a limitation thereto.

IV.A. Synthesis of Intermediate 1



Formation of Intermediate 1 follows the procedure described by Stout (Stout, (1983) *J. Med. Chem.* 26(6) : 808-13). To 4-methoxybenzyl amine (25g, 0.18 mol; Aldrich) is added 46% HBr in H_2O (106ml, 0.9 mol; Aldrich). The reaction is refluxed overnight, then the reaction is cooled to 0°C and neutralized to pH7 slowly with $KOH_{(s)}$. The reaction is allowed to stir for ~30 min, then the solid filtered and dried. The solid is redisolved in hot MeOH, filtered and the solution cooled to afford 19g (85%) intermediate 1.

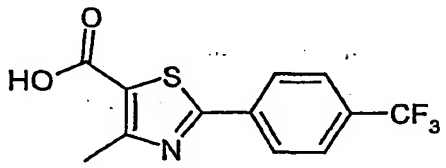
IV.B. Synthesis of Intermediate 2



A solution of ethyl 2-chloroacetoacetate (35.3g, 29.7mL, 0.21 mol) and 4-(trifluoromethyl)thiobenzamide (44g, 0.21 mol) in EtOH (300mL) is refluxed overnight. After cooling to room temperature the solvent is removed *in vacuo*.

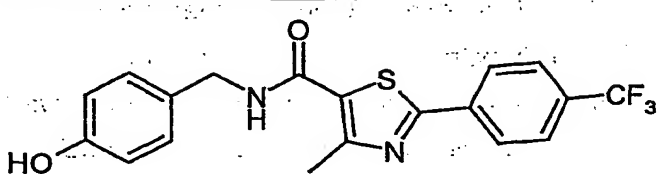
The final product (Intermediate 2) is recrystallized from a minimum of MeOH to afford 40g (59%) of final product as a white solid.

IV.C. Synthesis of Intermediate 3



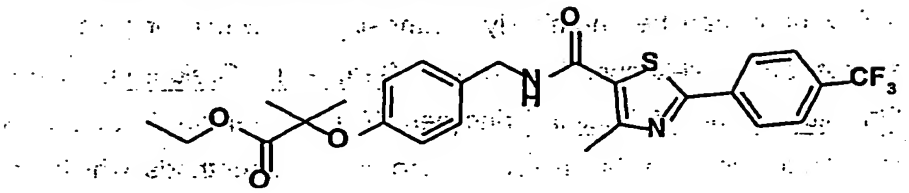
To Intermediate 2 (1.84g, 5.8 mmol) in THF is added 1N LiOH (6mL, 6 mmol) and the reaction stirred at room temperature. After ~3h, the reaction is neutralized with 1N HCl, extracted 3 x 100 mL EtOAc, dried over Na_2SO_4, filtered and the solvent removed under vaccum to afford 1.5g (89%) of Intermediate 3 as a white solid.

IV.D. Synthesis of Intermediate 4



To intermediate 3 (1g, 7 mmol) in CH_2Cl_2/DMF (1:1) is added HOBT (565mg, 4.2 mmol; Aldrich), EDC (800mg, 4.2 mmol; Aldrich) and Intermediate 1 (860mg, 7 mmol). The reaction is stirred at room temperature for 18h. The solvent is then removed *in vacuo*, treated with H_2O and extracted 3x 100mL CH_2Cl_2. The organic phases are then combined and washed with 1N HCl, dried over Na_2SO_4, filtered and evaporated to afford a mixture (*N*-substituted and *N,O*-substituted). The mixture is disolved in MeOH and treated with 1N NaOH. The reaction is stirred 18h at 50°C. The solvent removed *in vacuo*, dissolved in CH_2Cl_2, washed with H_2O, and dried over Na_2SO_4. The solvent evaporated the residue chromatographed (CH_2Cl_2/MeOH: 99/1) to afford 610mg (47%) of Intermediate 4 as a white solid.

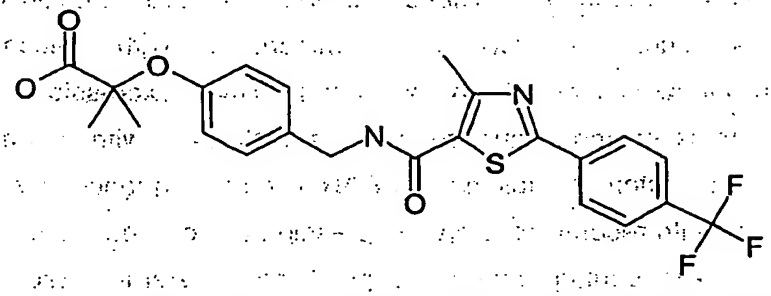
IV.E. Synthesis of Intermediate 5



2-methyl-2-[4-{[(4-methyl-2-[4-trifluoromethylphenyl]thiazol-5 ylcarbonyl)amino]methyl}phenoxy]propionic acid ethyl ester

To Intermediate 4 (710mg, 1.81 mmol) in DMF (50mL) is added the K_2CO_3 (275mg, 1.99 mmol) followed by the ethyl 2-bromo-2-methylpropanate (280µL, 1.91 mmol; Aldrich) and the reaction is heated to 80°C. After 18h, the reaction is cooled to room temperature and the solvent removed *in vacuo*. The residue is treated with water (200 mL), extracted 3 x 50mL CH_2Cl_2, dried over Na_2SO_4, filtered and the solvent removed under vaccum to afford 680mg (77%) of Intermediate 5 as a clear oil.

IV.F. Synthesis of Compound 1



2-methyl-2-[4-{[(4-methyl-2-[4-trifluoromethylphenyl]-thiazol-5-ylcarbonyl)amino]methyl}phenoxy]propionic acid

To Intermediate 5 (680mg, 1.39 mmol) in MeOH is added 1N NaOH (1.6 mL, 1.6 mmol) and the reaction is stirred at 60°C. After 18h, the reaction is cooled to room temperature and the solvent evaporated. The residue treated with 1N HCl, extracted 3 x 20 mL THF and the solvent is removed under vacuum to afford 500mg (75%) of Compound 1.

V. Production of PPAR Polypeptides

The native and mutated PPAR polypeptides, and fragments thereof, of the present invention can be chemically synthesized in whole or part using techniques that are well-known in the art (See, e.g., Creighton, (1983) Proteins: Structures and Molecular Principles, W.H. Freeman & Co., New York, incorporated herein in its entirety). Alternatively, methods which are well known to those skilled in the art can be used to construct expression vectors containing a partial or the entire native or mutated PPAR polypeptide coding sequence and appropriate transcriptional/translational control signals. These methods include *in vitro* recombinant DNA techniques, synthetic techniques and *in vivo* recombination/genetic recombination. See, for example, the techniques described throughout Sambrook et al., (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, New York, and Ausubel et al., (1989) Current Protocols in Molecular Biology, Greene Publishing Associates and Wiley Interscience, New York, both incorporated herein in their entirety.

A variety of host-expression vector systems can be utilized to express a PPAR coding sequence. These include but are not limited to microorganisms such as bacteria transformed with recombinant bacteriophage DNA, plasmid DNA or cosmid DNA expression vectors containing a PPAR coding sequence; yeast transformed with recombinant yeast expression vectors containing a PPAR coding sequence; insect cell systems infected with recombinant virus expression vectors (e.g., baculovirus) containing a PPAR coding sequence; plant cell systems infected with recombinant virus expression vectors (e.g., cauliflower mosaic virus, CaMV; tobacco mosaic virus, TMV) or transformed with recombinant plasmid expression vectors (e.g., Ti plasmid) containing a PPAR coding sequence; or animal cell systems. The expression elements of these systems vary in their strength and specificities.

Depending on the host/vector system utilized, any of a number of suitable transcription and translation elements, including constitutive and inducible promoters, can be used in the expression vector. For example, when cloning in bacterial systems, inducible promoters such as pL of

bacteriophage λ, plac, ptrp, ptac (ptrp-lac hybrid promoter) and the like can be used. When cloning in insect cell systems, promoters such as the baculovirus polyhedrin promoter can be used. When cloning in plant cell systems, promoters derived from the genome of plant cells, such as heat shock promoters; the promoter for the small subunit of RUBISCO; the promoter for the chlorophyll a/b binding protein) or from plant viruses (e.g., the 35S RNA promoter of CaMV; the coat protein promoter of TMV) can be used. When cloning in mammalian cell systems, promoters derived from the genome of mammalian cells (e.g., metallothionein promoter) or from mammalian viruses (e.g., the adenovirus late promoter; the vaccinia virus 7.5K promoter) can be used. When generating cell lines that contain multiple copies of the tyrosine kinase domain DNA, SV40-, BPV- and EBV-based vectors can be used with an appropriate selectable marker.

VI. Formation of PPARα Ligand Binding Domain Crystals

In one embodiment, the present invention provides crystals of PPARα LBD. The crystals were obtained using the methodology disclosed in the Examples. The PPARα LBD crystals, which can be native crystals, derivative crystals or co-crystals, have orthorhombic unit cells (an orthorhombic unit cell is a unit cell wherein $a \neq b \neq c$, and wherein $\alpha = \beta = \gamma = 90°$) and space group symmetry $P2_12_12$. There is one PPARα LBD molecule in the asymmetric unit. In this PPARα crystalline form, the unit cell has dimensions of a= 61.3 Å, b= 103.5 Å, c= 49.9 Å, and $\alpha = \beta = \gamma = 90°$. This crystal form can be formed in a crystallization reservoir comprising 4-8% PEG 3350, 100-200mM NaF, and 12-16% 2,5 hexanediol.

In another PPARα crystal form, the unit cell has dimensions of a = 95.58 Å, b = 122.06 Å, c = 122.10 Å, $\alpha = \beta = \gamma = 90°$ and belongs to the space group $P2_12_12_1$. There are four PPARα LBD molecules in the asymmetric unit of this crystal form. This crystal form can be formed in a crystallization reservoir comprising 50 mM bis-tris-propane, 4-6% PEG 3350, 150 mM $NaNO_3$, 16% 2,5 hexanediol, and 1-3 mM YCl_3.

VI.A. Preparation of PPAR Crystals

The native and derivative co-crystals, and fragments thereof, disclosed in the present invention can be obtained by a variety of techniques, including batch, liquid bridge, dialysis, vapor diffusion and hanging drop methods (See, e.g., McPherson, (1982) Preparation and Analysis of Protein Crystals, John Wiley, New York.; McPherson, (1990) *Eur. J. Biochem.* 189:1-23.; Weber, (1991) *Adv. Protein Chem.* 41:1-36). In a preferred embodiment, the vapor diffusion and hanging drop methods are used for the crystallization of PPAR polypeptides and fragments thereof.

In general, native crystals of the present invention are grown by dissolving substantially pure PPAR polypeptide or a fragment thereof in an aqueous buffer containing a precipitant at a concentration just below that necessary to precipitate the protein. Water is removed by controlled evaporation to produce precipitating conditions, which are maintained until crystal growth ceases.

In a preferred embodiment of the invention, native crystals are grown by vapor diffusion (See, e.g., McPherson, (1982) Preparation and Analysis of Protein Crystals, John Wiley, New York.; McPherson, (1990) *Eur. J. Biochem.* 189:1-23). In this method, the polypeptide/precipitant solution is allowed to equilibrate in a closed container with a larger aqueous reservoir having a precipitant concentration optimal for producing crystals. Generally, less than about 25 μL of PPAR polypeptide solution is mixed with an equal volume of reservoir solution, giving a precipitant concentration about half that required for crystallization. This solution is suspended as a droplet underneath a coverslip, which is sealed onto the top of the reservoir. The sealed container is allowed to stand, until crystals grow. Crystals generally form within two to six weeks, and are suitable for data collection within approximately seven to ten weeks. Of course, those of skill in the art will recognize that the above-described crystallization procedures and conditions can be varied.

VI.B. Preparation of Derivative Crystals

Derivative crystals of the present invention, e.g. heavy atom derivative crystals, can be obtained by soaking native crystals in mother liquor containing salts of heavy metal atoms. Such derivative crystals are useful for phase analysis in the solution of crystals of the present invention. In a preferred embodiment of the present invention, for example, soaking a native crystal in a solution containing methyl-mercury chloride provides derivative crystals suitable for use as isomorphous replacements in determining the X-ray crystal structure of a PPAR polypeptide. Additional reagents useful for the preparation of the derivative crystals of the present invention will be apparent to those of skill in the art after review of the disclosure of the present invention presented herein.

VI.C. Preparation of Co-crystals

Co-crystals of the present invention can be obtained by soaking a native crystal in mother liquor containing compounds known or predicted to bind the LBD of a PPAR, or a fragment thereof. Alternatively, co-crystals can be obtained by co-crystallizing a PPAR LBD polypeptide or a fragment thereof in the presence of one or more compounds known or predicted to bind the polypeptide. In a preferred embodiment, such a compound is Compound 1.

VI.D. Solving a Crystal Structure of the Present Invention

Crystal structures of the present invention can be solved using a variety of techniques including, but not limited to, isomorphous replacement, anomalous scattering or molecular replacement methods. Computer software packages will also be helpful in solving a crystal structure of the present invention. Applicable software packages include but are not limited to X-PLOR™ program (Brünger, (1992) *X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR*, Yale University Press, New Haven, Connecticut; X-PLOR is available from Molecular Simulations, Inc., San Diego, California), Xtal View (McRee, (1992) *J. Mol. Graphics* 10: 44-47; X-tal View is available from the San Diego Supercomputer Center). SHELXS 97 (Sheldrick (1990) *Acta Cryst.* A46: 467; SHELX 97 is available from the Institute of Inorganic

Chemistry, Georg-August-Universität, Göttingen, Germany), HEAVY (Terwilliger, Los Alamos National Laboratory) and SHAKE-AND-BAKE (Hauptman, (1997) *Curr. Opin. Struct. Biol.* 7: 672-80; Weeks et al., (1993) *Acta Cryst.* D49: 179; available from the Hauptman-Woodward Medical Research Institute, Buffalo, New York) can be used. See also, Ducruix & Geige, (1992) Crystallization of Nucleic Acids and Proteins: A Practical Approach, IRL Press, Oxford, England, and references cited therein.

VII. Characterization and Solution of a PPARα Ligand Binding Domain Crystal

VII.A Unique Structural Differences Between PPARα and Other PPARs

The PPARα LBD-ligand structure was solved here using molecular replacement techniques. The overall folding of the protein backbone, and the binding mode of Compound 1, are shown in the ribbon diagram of Figure 1. Specific interactions between Compound 1 and the protein are shown schematically in Figure 2. The structure of the PPARγ LBD was solved previously in the apo form, i.e., with no ligand, and also with a thiazolidinedione ligand (rosiglitazone) and a coactivator peptide (Nolte et al., (1998) *Nature* 395:137-43). The apo structure has also been determined independently (Uppenberg et al., (1998) *J. Biol. Chem.* 273: 31108-12). In addition, the structure of the PPARγ LBD has been determined with a partial agonist, GW0072 (Oberfield et al., (1999) *Proc. Nat. Acad. Sci.* 96: 6102-106). The structure of the PPARγ LBD has also been determined in the heterodimeric complex with RXRα, together with coactivator peptides, with rosiglitazone, and also with a carboxylic acid ligand, GI262570 (Gampe et al., (2000) *Mol. Cell* 5: 545-55). The structure of the PPARδ LBD has been determined in the apo form, and with eicosapentaenoic acid, and with the synthetic compound GW2433 (Xu et al., (1999) *Mol. Cell* 3: 397-403).

To facilitate comparison, the structures were first translated and rotated into a common position and orientation as shown in Figure 1. This superimposition operation was done with the MVP program (Lambert, (1997) in Practical Application of Computer–Aided Drug Design, (Charifson, ed.), pp. 243-303, Marcel-Dekker, New York) by first aligning the amino acid sequences to identify corresponding residues in the three different PPARs, and then rotating and translating so as to superimpose corresponding C_α or backbone atoms from the aligned residues. With this translation and rotation, most of the major alpha-helices and beta-strands of the three PPARs are closely superimposed. The AF2 helix is well superimposed in most of the structures, but is shifted into a different position in certain subunits of structures of PPARγ either in the absence of ligand (apo), or in the presence of the partial agonist GW0072. This shift provides evidence that the PPAR AF2 helix can shift out of the active conformation, and that it is more likely to do so in the absence of a strongly activating ligand. In the above listed PPAR X-ray structures, the ligands that act as strong agonists (rosiglitazone, GI262570, eicosapentaenoic acid, GW2433, Compound 1) are all oriented with the acid group near the AF2 helix, and they all make a hydrogen bond with a tyrosine residue in the AF2 helix (Tyr464 in PPARα, Tyr473 in PPARγ, Tyr437 in PPARδ). The partial agonist, GW0072, also has a carboxyl group, but it is oriented differently, and fails to make any hydrogen bond with the AF2 tyrosine. This suggests that the hydrogen bond between the ligand and the AF2 tyrosine helps to hold the AF2 helix in the active conformation and thereby facilitate coactivator binding. See, Xu et al., (1999) *Mol. Cell* 3: 397-403 and Oberfield et al., (1999) *Proc. Nat. Acad. Sci.* 96: 6102-106.

To facilitate discussion, it is useful to establish a nomenclature for regions of the ligand and the ligand binding pocket. The strongly activating ligands in these X-ray structures all have an acid group that binds near the AF2 tyrosine, and a lipophilic "tail" that extends into a lipophilic pocket. The acid group can be called the acid "headgroup", and the site near the AF2 helix into which it binds can be called the "headgroup binding site". In rosiglitazone, GI262570 and Compound 1, the lipophilic tail is directed into a lipophilic

pocket delineated by helix-2', helix-3 and the beta sheet. This will be called the "lower tail pocket" or "lower pocket". In the structure of PPARδ bound to eicosapentaenoic acid, the eicosapentaenoic acid was found in two different binding modes with roughly equal occupancy (Xu et al., (1999) *Mol. Cell* 3: 397-403). In both binding modes, the acid headgroup bound in the headgroup binding site near Tyr 437. In one binding mode, the lipophilic tail was directed into the lower tail pocket. However, in the other binding mode, the lipophilic tail was directed into a different pocket, delineated by helix-3, helix-5, the beta sheet and the loop between helix-1 and helix-2. This will be called the "upper tail pocket." GW2433 has a branched tail, and was found to bind with one branch in the lower pocket, and with the other branch in the upper pocket (Xu et al., (1999) *Mol. Cell* 3: 397-403). GI262570 has an additional lipophilic benzophenone group near the acid headgroup. This benzophenone group was found to be directed into a lipophilic pocket delineated by helix-3, helix-7, helix-10 and the loop between helix-10 and the AF2 helix. This will be subsequently referred to as the "benzophenone pocket."

Comparing the backbone structures, there are substantial differences between PPARα, PPARγ and PPARδ in the "loop" region between helix-2 and strand-1, the loop region between helix-2' and helix-3, and the loop region between helix-10 and the AF2 helix. There are also smaller differences in the loop region between helix-1 and helix-2, and the loop region between helix-6 and helix-7. Helices 2, 2' and 3' are closely superimposed, but have slightly different lengths, as indicated in Table 4. Helix-10 has the same length in all structures, but bends differently over the ligand binding pocket in PPARα, PPARγ and PPARδ. Some of these structural differences are visible in Figure 3. Many of these structural differences lie close to the ligand binding pocket, and could therefore be important in the receptor selectivity of different ligands.

Helix-2' and the loop between helix-2' and helix-3 (the 2'-3 loop) together serve as one wall for the "lower tail pocket" in all three PPARs. Helix-2', and the 2'-3 loop, adopt different conformations in some of the different PPARγ structures. In particular, helix-2' is shorter in the homodimer

structures of PPARγ bound to rosiglitazone and GW0072, and in the absence of ligand, than it is in the RXRα/PPARγ heterodimer structures where PPARγ is bound to rosiglitazone or GI262570. Some of these conformational differences might result from differences in crystal packing. However, the RXRα/PPARγ heterodimer represents the closer approximation to the biologically active complex, and will be used here to represent the most relevant conformation of PPARγ. By contrast, helix-2' and the 2'-3 loop adopt more nearly equivalent backbone conformations in the available X-ray structures of PPARα and PPARδ. Considering the conformation in the RXRα/PPARγ/GI262570 heterodimer structure, helix-2' is longer in PPARα and PPARδ, and the C-terminal end of the helix adopts different conformations in the three PPARs. In PPARα, the last residue of the helix, Leu254, makes the expected alpha-helical hydrogen bonds, but bulges away from the axis of the helix towards the ligand. This bulged conformation allows Leu254 and Val255 to cover the "bottom" of the lower tail pocket, effectively narrowing the mouth of the pocket. In PPARδ, the C-terminal end of helix-2' is wound more loosely, such that the corresponding residue, Leu226, cannot cover the bottom of the ligand binding pocket. Instead, the 2'-3 loop adopts a different conformation that places the side-chain of Trp228 in the bottom of the lower tail pocket. This shortens the lower tail pocket slightly, and also constricts the opening to solvent. In PPARγ, helix-2' is bent such that its corresponding residue, Ile262, is shifted farther from the pocket. Also, the next two residues, Lys263 and Phe264, adopt the helical conformation, effectively extending helix-2 by two residues, such that Lys263 is far from the ligand and cannot cover the solvent channel. This leaves a very wide opening to solvent at this position in PPARγ, as depicted by the large, wide cavity region above the 2'-3 loop in Figure 5. The opening is much narrower in PPARα and PPARδ, as depicted in Figures 4 and 6. These variations in the backbone conformation would be difficult or impossible to predict from the previously available X-ray structures with any homology modeling procedure. Nonetheless, very accurate models for helix-2' and the 2'-3 loop in all three

PPARs would be essential for understanding the binding mode and receptor selectivity of ligands that occupy the lower tail pocket.

The loop between helix-1 and helix-2 (the "1-2 loop") serves as a wall at the far end of the upper tail pocket. Residues in this 1-2 loop come close to the tail of eicosapentaenoic acid (in its upper tail pocket binding mode), and close to the fluoro-,chloro-phenyl ring of GW2433 in PPARδ. Several backbone amide CO and NH groups are directed towards the ligand binding site, and could serve as hydrogen bonding partners with an appropriately designed ligand. However, the backbone conformation in the 1-2 loop is slightly different in PPARα, PPARγ and PPARδ. In particular, the backbone amide CO and NH groups have slightly different orientations in PPARα, PPARγ and PPARδ. Some of these differences may result from the presence of a proline at position 227 in PPARγ, whereas PPARα and PPARδ have asparagines at this position. These subtle differences would be difficult or impossible to predict to high accuracy using the previously available X-ray structures with standard homology modeling procedures. Nonetheless, a very accurate model of this loop conformation would be essential for understanding the receptor selectivity of ligands that interact with this loop.

The C-terminal end of helix-10 and the loop between helix-10 and the AF2 helix (the "10-AF2 loop") together serve as one wall for the headgroup binding site and the benzophenone pocket. An additional wall is provided by a glutamine residue in helix-3 (Gln277 in PPARα, Gln286 in PPARγ, Gln250 in PPARδ) that reaches across the benzophenone binding site to make hydrogen bonds with backbone CO and NH groups from the 10-AF2 loop. This glutamine side-chain, and the 10-AF2 loop itself, adopt different conformations in the three PPARs. In PPARα and PPARδ, the glutamine side-chain adopts conformations that narrow the benzophenone pocket substantially. In addition, in PPARα and PPARδ, the 10-AF2 loop adopts a conformation that crowds a phenylalanine from helix-3 (Phe273 in PPARα, Phe282 in PPARγ, Phe246 in PPARδ) more in PPARα and PPARδ than in PPARγ. These two structural differences cause a slight narrowing of the

benzophenone pocket in PPARα, and a more substantial narrowing in PPARδ. This can be seen by comparison of PPARα and PPARδ in Figures 4 and 6 with PPARγ in Figure 5. The narrowing is sufficient to significantly reduce the binding affinity of ligands that have a benzophenone group at this position. The narrowing in PPARα and PPARδ suggests that smaller groups should be used at this position to obtain good binding to PPARα, and substantially smaller groups should be used to obtain good binding to PPARδ. Aside from these changes that narrow the pocket in PPARα and PPARδ, there are also structural changes that modulate the shape of the pocket and the position and orientation of potential hydrogen bonding groups. For example, the C-terminal end of helix-10 bends inwards toward the ligand binding site in all three PPARs. However, the bend is slightly different in the different PPARs, placing corresponding side-chains in slightly different positions. These variations in the backbone conformation, and corresponding changes in side-chain conformation, would be difficult or impossible to predict from the previously available X-ray structures with any available homology modeling procedure. Nonetheless, very accurate models for helix-10, the 10-AF2 loop and the side-chains in this region would be essential for understanding the binding mode and receptor selectivity of ligands that occupy the benzophenone pocket.

Aside from these unexpected differences in the backbone structure of PPARα, the present X-ray structure also revealed differences involving side-chains. In some cases, these differences involve residue positions where the amino acid is different in PPARα from that in either PPARγ or PPARδ or both. In other cases, PPARα may have the same amino acid at a particular residue position as PPARγ or PPARδ or both, but the amino acid side-chain adopts a different conformation in PPARα.

One of the most important side-chain differences is Tyr314 in PPARα, a position that corresponds to His323 in PPARγ and His287 in PPARδ. In PPARγ and PPARδ, this histidine residue makes a hydrogen bond with the acidic headgroup of the ligand for all strongly activating ligands for which

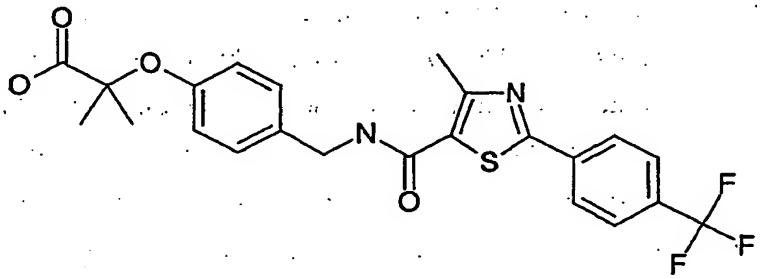
structures are available. The present PPARα structures shows that Tyr314 also makes a hydrogen bond with the acidic headgroup of Compound 1. However, the tyrosine OH lies farther from the protein backbone than the corresponding hydrogen bonding atoms in histidine. Consequently, changing histidine to tyrosine could potentially require a change in the position and/or orientation and/or conformation of the ligand, or changes in the conformation of the PPARα protein. The present PPARα crystal structure showed that the protein backbone is essentially unchanged in this region of PPARα, compared with PPARγ and PPARδ. Instead, the acid headgroup of the ligand is shifted and rotated in such a way that it can still make hydrogen bonds with Ser280, Tyr314, His440 and Tyr464. This involves small changes in the conformations of Tyr314, His440 and Tyr464, relative to PPARγ and PPARδ. Also, this involves a larger change in the conformation of Ser280, which unexpectedly adopts a conformation different from that of Ser289 in PPARγ bound to GI262570. The PPARα conformation places the Ser280 side-chain oxygen near the position of the side-chain oxygen of Thr253 in PPARδ bound to GW2433. The exact shift and rotation, and the exact conformations of the side-chains of Ser280, Tyr314, His440 and Tyr464, would be difficult or impossible to predict without this X-ray crystal structure of PPARα. However, this shift and rotation do significantly affect the position of the whole ligand within the ligand binding site. The position and orientation of the ligand carboxylate group revealed in this PPARα X-ray structure, and the interactions it makes with Ser280, Tyr314, His440 and Tyr464, can serve as a template for docking other compounds into PPARα using molecular modeling procedures.

This PPARα X-ray structure also revealed numerous other side-chains where the conformation in PPARα was different from that in PPARγ and/or PPARδ, and where the diffence could affect the shape of the ligand binding pocket, and the position, orientation and/or conformation of the ligand. These additional residues with differences include, but are not limited to, Gln277, Phe273, His274, Ile354, Leu321, Met320, Met330 and Glu251. The side-

chain conformational differences involving Gln277, Phe273 and Ile354 affect the volume and detailed shape of the headgroup binding site and/or the benzophenone pocket. His274 may affect these pockets indirectly, through its effect on Gln277 and Phe273. Leu321, Met320, Met330 and Glu251 affect the shape and volume of the upper and lower tail pockets. Numerous other side-chains also affect the size, shape and electrostatic character of the ligand binding site, and the position, orientation and conformation of the ligand within the ligand binding site. An understanding of the PPARα, PPARγ and PPARδ selectivity of various ligands would depend on having an accurate structure of each of the three PPARs, as well as an accurate position of the whole ligand within the pocket. This PPARα X-ray structure provides an accurate protein structure, as well as a template for modeling alternative ligands.

VII.B Characterization of the PPARα Binding Pocket

The ligand binding domain of PPARα was co-crystallized with Compound 1, which has the IUPAC name 2-methyl-2-[4-{[(4-methyl-2-[4-trifluoromethylphenyl] thiazol-5-yl-carbonyl) amino] methyl} phenoxy] propionic acid.



Compound 1

Compound 1 is an agonist of hPPARα and is useful for treatment of hPPARα mediated diseases or conditions including dyslipidemia, syndrome X, heart failure, hypercholesteremia, cardiovascular disease, type II diabetes

mellitus, type I diabetes, insulin resistance, hyperlipidemia, obesity, inflammation, anorexia bulimia and anorexia nervosa.

Figures 1, 2 and 7 depict the conformation and orientation of the ligand Compound 1 in the binding site. Figure 1 depicts the overall orientation of the α helices and β strands of the ligand binding domain of PPARα as it binds Compound 1. Compound 1 is presented as a spacefilling model.

A more specific graphical description of the residues of the PPARα LBD involved in ligand binding is presented in Figure 2. Figure 2 is a schematic diagram depicting those residues of the PPARα LBD that interact with Compound 1 as it is bound in the binding pocket of the PPARα LBD. Note that Figure 2 is a schematic diagram, and highlights residues that interact with the ligand and does not indicate intermolecular distances.

VII.C. Hydrogen Bonding in the Binding Pocket of the PPARα LBD

The hydrogen bonding scheme of the solvated binding pocket is presented in Figure 7. In Figure 7, atoms are shaded according to element, with carbon, fluorine, nitrogen, oxygen, sulfur and hydrogen in progressively lighter shades of gray. Sulfur is depicted with a slightly bigger ball, while hydrogen, fluorine and oxygen are depicted with slightly smaller balls. The hydrogen atoms shown here were not visible in the electron density, and were instead modeled into reasonable conformations (using standard bond lenghts and angles) to obtain possible hydrogen bond interactions, shown here with strings of small white balls. Each interaction is annotated with its distance in angstroms. Residues of the PPARα LBD binding pocket involved in hydrogen bonding are labeled. It is observed that hydrogen bonding relationships exist between the side chains of PPARα LBD residues and the ligand, between the side chains of PPARα LBD residues and solvent molecules, and between the ligand and solvent molecules. The hydrogen bonding pairs are identified by dotted lines.

Figure 7 highlights hydrogen bonding that occurs between solvent molecules (indicated as crosses in Figure 7) and the side chains of PPARα

LBD residues in the binding pocket. Residues that hydrogen bond to solvent and are visible in Figure 7 include Ser-280, Ser-283, Thr-279 and Ala-333.

Additionally, Figure 7 highlights those residues of the PPARα LBD that hydrogen bond directly to the ligand. Residues of the PPARα LBD in which side chains hydrogen bond directly to the ligand are visible in Figure 7, and include His-440, Tyr-464, Tyr-314, Ser 280 and Thr-279.

VII.D. Generation of Easily-Solved PPAR Crystals

The present invention discloses a substantially pure PPAR LBD polypeptide in crystalline form. In a preferred embodiment, exemplified in the Figures and Laboratory Examples, PPARα is crystallized with bound ligand. Crystals are formed from PPAR LBD polypeptides that are usually expressed by a cell culture, such as *E. coli*. Bromo-, iodo- and substitutions can be included during the preparation of crystal forms and can act as heavy atom substitutions in PPAR ligands and crystals of PPARs. This method can be advantageous for the phasing of the crystal, which is a crucial, and sometimes limiting, step in solving the three-dimensional structure of a crystallized entity. Thus, the need for generating the heavy metal derivatives traditionally employed in crystallography can be eliminated. After the three-dimensional structure of a PPAR or PPAR LBD with or without a ligand bound is determined, the resultant three-dimensional structure can be used in computational methods to design synthetic ligands for PPARα and other PPAR polypeptides. Further activity structure relationships can be determined through routine testing, using assays disclosed herein and known in the art.

VIII. Uses of PPARα Crystals and the Three-Dimensional Structure of the Ligand Binding Domain of PPARα

VIII.A. Design and Development of PPAR Modulators

The knowledge of the structure of the PPARα ligand binding domain (LBD), an aspect of the present invention, provides a tool for investigating the

mechanism of action of PPARα and other PPAR polypeptides in a subject. For example, various computer modelleing programs, as described herein, can predict the binding of various ligand molecules to the LBD of PPARα, PPARγ or PPARδ. Upon discovering that such binding in fact takes place, knowledge of the protein structure then allows design and synthesis of small molecules that mimic the functional binding of the ligand to the LBD of PPARα, and to the LBDs of other PPAR polypeptides. This is the method of "rational" drug design, further described herein.

Use of the isolated and purified PPARα crystalline structure of the present invention in rational drug design is thus provided in accordance with the present invention. Additional rational drug design techniques are described in U.S. Patent Nos. 5,834,228 and 5,872,011, incorporated herein in their entirety.

Thus, in addition to the compounds described herein, other sterically similar compounds can be formulated to interact with the key structural regions of a PPAR in general, or of PPARα in particular. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

VIII.A.1. Rational Drug Design

The three-dimensional structure of ligand-binding PPARα is unprecedented and will greatly aid in the development of new synthetic ligands for a PPAR polypeptide, such as PPAR agonists and antagonists, including those that bind exclusively to any one of the PPAR subtypes. In addition, the PPARs are well suited to modern methods, including three-dimensional structure elucidation and combinatorial chemistry, such as those disclosed in U.S. Patent No. 5,463,564, incorporated herein by reference. Structure determination using X-ray crystallography is possible because of the solubility properties of the PPARs. Computer programs that use crystallography data when practicing the present invention will enable the

rational design of ligands to these receptors. Programs such as RASMOL (Biomolecular Structures Group, Glaxo Wellcome Research & Development Stevenage, Hertfordshire, UK Version 2.6, August 1995, Version 2.6.4, December 1998, Copyright © Roger Sayle 1992-1999) can be used with the atomic structural coordinates from crystals generated by practicing the invention or used to practice the invention by generating three-dimensional models and/or determining the structures involved in ligand binding. Computer programs such as those sold under the registered trademark INSIGHT II®, and such as GRASP (Nicholls et al., (1991) *Proteins* 11: 282) allow for further manipulations and the ability to introduce new structures. In addition, high throughput binding and bioactivity assays can be devised using purified recombinant protein and modern reporter gene transcription assays known to those of skill in the art in order to refine the activity of a designed ligand.

A method of identifying modulators of the activity of a PPAR polypeptide using rational drug design is thus provided in accordance with the present invention. The method comprises designing a potential modulator for a PPAR polypeptide of the present invention that will form non-covalent interactions with amino acids in the ligand binding pocket based upon the crystalline structure of the PPARα LBD polypeptide; synthesizing the modulator; and determining whether the potential modulator modulates the activity of the PPAR polypeptide. In a preferred embodiment, the modulator is designed for a PPARα polypeptide. Preferably, the PPARα polypeptide comprises the nucleic acid sequence of SEQ ID NO:1; and the PPARα LBD comprises the nucleic acid sequence SEQ ID NO:3. The determination of whether the modulator modulates the biological activity of a PPAR polypeptide is made in accordance with the screening methods disclosed herein, or by other screening methods known to those of skill in the art. Modulators can be synthesized using techniques known to those of ordinary skill in the art.

In an alternative embodiment, a method of designing a modulator of a PPAR polypeptide in accordance with the present invention is disclosed

comprising: (a) selecting a candidate PPAR ligand; (b) determining which amino acid or amino acids of an PPAR polypeptide interact with the ligand using a three-dimensional model of a crystallized PPARα LBD; (c) identifying in a biological assay for PPAR activity a degree to which the ligand modulates the activity of the PPAR polypeptide; (d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the PPAR polypeptide and the ligand is predicted to be modulated by the chemical modification; (e) performing the chemical modification on the ligand to form a modified ligand; (f) contacting the modified ligand with the PPAR polypeptide; (g) identifying in a biological assay for PPAR activity a degree to which the modified ligand modulates the biological activity of the PPAR polypeptide ; and (h) comparing the biological activity of the PPAR polypeptide in the presence of modified ligand with the biological activity of the PPAR polypeptide in the presence of the unmodified ligand, whereby a modulator of an PPAR polypeptide is designed.

VIII.A.2. Methods for Using the PPARα LBD Structural Coordinates For Molecular Design

For the first time, the present invention permits the use of molecular design techniques to design, select and synthesize chemical entities and compounds, including modulatory compounds, capable of binding to the ligand binding pocket or an accessory binding site of PPARα and the PPARα LBD, in whole or in part. Correspondingly, the present invention also provides for the application of similar techniques in the design of modulators of any PPAR polypeptide.

In accordance with a preferred embodiment of the present invention, the structure coordinates of a crystalline PPARα LBD can be used to design compounds that bind to a PPAR LBD (more preferably a PPARα LBD) and alter the properties of a PPAR LBD (for example, the dimerization or ligand binding ability) in different ways. One aspect of the present invention provides for the design of compounds that can compete with natural or engineered ligands of a PPAR polypeptide by binding to all, or a portion of, the binding

sites on a PPAR LBD. The present invention also provides for the design of compounds that can bind to all, or a portion of, an accessory binding site on a PPAR that is already binding a ligand. Similarly, non-competitive agonists/ligands that bind to and modulate PPAR LBD activity, whether or not it is bound to another chemical entity, can be designed using the PPAR LBD structure coordinates of this invention.

A second design approach is to probe a PPAR or PPAR LBD (preferably a PPARα or PPARα LBD) crystal with molecules comprising a variety of different chemical entities to determine optimal sites for interaction between candidate PPAR or PPAR LBD modulators and the polypeptide. For example, high resolution X-ray diffraction data collected from crystals saturated with solvent allows the determination of the site where each type of solvent molecule adheres. Small molecules that bind tightly to those sites can then be designed and synthesized and tested for their PPARα modulator activity. Representative designs are also disclosed in published PCT application WO 99/26966.

Once a computationally-designed ligand is synthesized using the methods of the present invention or other methods known to those of skill in the art, assays can be used to establish its efficacy of the ligand as a modulator of PPAR (preferably PPARα) activity. After such assays, the ligands can be further refined by generating intact PPAR, or PPAR LBD, crystals with a ligand bound to the LBD. The structure of the ligand can then be further refined using the chemical modification methods described herein and known to those of skill in the art, in order to improve the modulation activity or the binding affinity of the ligand. This process can lead to second generation ligands with improved properties.

Ligands also can be selected that modulate PPAR responsive gene transcription by the method of altering the interaction of co-activators and co-repressors with their cognate PPAR. For example, agonistic ligands can be selected that block or dissociate a co-repressor from interacting with the PPAR, and/or that promote binding or association of a co-activator. Antagonistic ligands can be selected that block co-activator interaction and/or

promote co-repressor interaction with a target receptor. Selection can be done via binding assays that screen for designed ligands having the desired modulatory properties. Preferably, interactions of a PPARα polypeptide are targeted. Suitable assays for screening that can be employed, *mutatis mutandis* in the present invention, are described in as described in Nichols et al., (1998) *Anal. Biochem.* 257: 112-19 and Xu et al., (1999) *Mol. Cell* 3: 397-403, which are incorporated herein in their entirety by reference.

VIII.A.3. Methods of Designing PPARα LBD Modulator Compounds

The design of candidate substances, also referred to as "compounds" or "candidate compounds", that bind to or inhibit PPAR LBD-mediated activity according to the present invention generally involves consideration of two factors. First, the compound must be capable of physically and structurally associating with a PPAR LBD. Non-covalent molecular interactions important in the association of a PPAR LBD with its substrate include hydrogen bonding, van der Waals interactions and hydrophobic interactions.

Second, the compound must be able to assume a conformation that allows it to associate with a PPAR LBD. Although certain portions of the compound will not directly participate in this association with a PPAR LBD, those portions can still influence the overall conformation of the molecule. This, in turn, can have a significant impact on potency. Such conformational requirements include the overall three-dimensional structure and orientation of the chemical entity or compound in relation to all or a portion of the binding site, e.g., the ligand binding pocket or an accessory binding site of a PPAR LBD, or the spacing between functional groups of a compound comprising several chemical entities that directly interact with a PPAR LBD.

The potential modulatory or binding effect of a chemical compound on a PPAR LBD can be analyzed prior to its actual synthesis and testing by the use of computer modeling techniques that employ the coordinates of a crystalline PPARα LBD polypeptide of the present invention. If the theoretical structure of the given compound suggests insufficient interaction and

association between it and a PPAR LBD, synthesis and testing of the compound is obviated. However, if computer modeling indicates a strong interaction, the molecule can then be synthesized and tested for its ability to bind and modulate the activity of a PPAR LBD. In this manner, synthesis of unproductive or inoperative compounds can be avoided.

A modulatory or other binding compound of a PPAR LBD polypeptide (preferably a PPARα LBD) can be computationally evaluated and designed via a series of steps in which chemical entities or fragments are screened and selected for their ability to associate with the individual binding sites or other areas of a crystalline PPARαLBD polypeptide of the present invention.

One of several methods can be used to screen chemical entities or fragments for their ability to associate with a PPAR LBD and, more particularly, with the individual binding sites of a PPAR LBD, such as ligand binding pocket or an accessory binding site. This process can begin by visual inspection of, for example, the ligand binding pocket on a computer screen based on the PPARα LBD atomic coordinates in Table 2. Selected fragments or chemical entities can then be positioned in a variety of orientations, or docked, within an individual binding site of a PPARα LBD as defined herein above. Docking can be accomplished using software programs such as those available under the tradenames QUANTA™ (Molecular Simulations Inc., San Diego, California) and SYBYL™ (Tripos, Inc., St. Louis, Missouri), followed by energy minimization and molecular dynamics with standard molecular mechanics forcefields, such as CHARM (Brooks et al., (1983) *J. Comp. Chem.*, 8: 132) and AMBER 5 (Case et al., (1997), AMBER 5, University of California, San Francisco; Pearlman et al., (1995) *Comput. Phys. Commun.* 91: 1-41).

Specialized computer programs can also assist in the process of selecting fragments or chemical entities. These include:

1. GRID™ program, version 17 (Goodford, (1985) *J. Med. Chem.* 28: 849-57), which is available from Molecular Discovery Ltd., Oxford, UK;

2. MCSS™ program (Miranker & Karplus, (1991) *Proteins* 11: 29-34), which is available from Molecular Simulations, Inc., San Diego, California;

3. AUTODOCK™ 3.0 program (Goodsell & Olsen, (1990) *Proteins* 8: 195-202), which is available from the Scripps Research Institute, La Jolla, California;

4. DOCK™ 4.0 program (Kuntz et al., (1992) *J. Mol. Biol.* 161: 269-88), which is available from the University of California, San Francisco, California;

5. FLEX-X™ program (See, Rarey et al., (1996) *J. Comput. Aid. Mol. Des.* 10:41-54), which is available from Tripos, Inc., St. Louis, Missouri;

6. MVP program (Lambert, (1997) in Practical Application of Computer-Aided Drug Design, (Charifson, ed.) Marcel-Dekker, New York, pp. 243-303); and

7. LUDI™ program (Bohm, (1992) *J. Comput. Aid. Mol. Des.*, 6: 61-78), which is available from Molecular Simulations, Inc., San Diego, California.

Once suitable chemical entities or fragments have been selected, they can be assembled into a single compound or modulator. Assembly can proceed by visual inspection of the relationship of the fragments to each other on the three-dimensional image displayed on a computer screen in relation to the structure coordinates of a PPARα LBD. Manual model building using software such as QUANTA™ or SYBYL™ typically follows.

Useful programs to aid one of ordinary skill in the art in connecting the individual chemical entities or fragments include:

1. CAVEAT™ program (Bartlett et al., (1989) *Special Pub., Royal Chem. Soc.* 78: 182-96), which is available from the University of California, Berkeley, California;

2. 3D Database systems, such as MACCS-3D™ system program, which is available from MDL Information Systems, San Leandro, California. This area is reviewed in Martin, (1992) *J. Med. Chem.* 35: 2145-54; and

3. HOOK™ program (Eisen et al., (1994). *Proteins* 19: 199-221), which is available from Molecular Simulations, Inc., San Diego, California.

Instead of proceeding to build a PPAR LBD modulator (preferably a PPARα LBD modulator) in a step-wise fashion one fragment or chemical entity at a time as described above, modulatory or other binding compounds

can be designed as a whole or *de novo* using the structural coordinates of a crystalline PPARα LBD polypeptide of the present invention and either an empty binding site or optionally including some portion(s) of a known modulator(s). Applicable methods can employ the following software programs:

1. LUDI™ program (Bohm, (1992) *J. Comput. Aid. Mol. Des.*, 6: 61-78), which is available from Molecular Simulations, Inc., San Diego, California;

2. LEGEND™ program (Nishibata & Itai, (1991) *Tetrahedron* 47: 8985); and

3. LEAPFROG™, which is available from Tripos Associates, St. Louis, Missouri.

Other molecular modeling techniques can also be employed in accordance with this invention. See, e.g., Cohen et al., (1990) *J. Med. Chem.* 33: 883-94. See also, Navia & Murcko, (1992) *Curr. Opin. Struc. Biol.* 2: 202-10; U.S. Patent No. 6,008,033, herein incorporated by reference.

Once a compound has been designed or selected by the above methods, the efficiency with which that compound can bind to a PPARα LBD can be tested and optimized by computational evaluation. By way of particular example, a compound that has been designed or selected to function as a PPARα LBD modulator should also preferably traverse a volume not overlapping that occupied by the binding site when it is bound to its native ligand. Additionally, an effective PPAR LBD modulator should preferably demonstrate a relatively small difference in energy between its bound and free states (i.e., a small deformation energy of binding). Thus, the most efficient PPAR LBD modulators should preferably be designed with a deformation energy of binding of not greater than about 10 kcal/mole, and preferably, not greater than 7 kcal/mole. It is possible for PPAR LBD modulators to interact with the polypeptide in more than one conformation that is similar in overall binding energy. In those cases, the deformation energy of binding is taken to be the difference between the energy of the free compound and the average energy of the conformations observed when the modulator binds to the polypeptide.

A compound designed or selected as binding to a PPAR polypeptide (preferably a PPARα LBD polypeptide) can be further computationally optimized so that in its bound state it would preferably lack repulsive electrostatic interaction with the target polypeptide. Such non-complementary (e.g., electrostatic) interactions include repulsive charge-charge, dipole-dipole and charge-dipole interactions. Specifically, the sum of all electrostatic interactions between the modulator and the polypeptide when the modulator is bound to a PPAR LBD preferably make a neutral or favorable contribution to the enthalpy of binding.

Specific computer software is available in the art to evaluate compound deformation energy and electrostatic interaction. Examples of programs designed for such uses include:

1. Gaussian 98™, which is available from Gaussian, Inc., Pittsburgh, Pennsylvania;

2. AMBER™ program, version 6.0, which is available from the University of California at San Francisco;

3. QUANTA™ program, which is available from Molecular Simulations, Inc., San Diego, California;

4. CHARMm® program, which is available from Molecular Simulations, Inc., San Diego, California; and

4. Insight II® program, which is available from Molecular Simulations, Inc., San Diego, California.

These programs can be implemented using a suitable computer system. Other hardware systems and software packages will be apparent to those skilled in the art after review of the disclosure of the present invention presented herein.

Once a PPAR LBD modulating compound has been optimally selected or designed, as described above, substitutions can then be made in some of its atoms or side groups in order to improve or modify its binding properties. Generally, initial substitutions are conservative, i.e., the replacement group will have approximately the same size, shape, hydrophobicity and charge as the original group. It should, of course, be understood that components

known in the art to alter conformation should be avoided. Such substituted chemical compounds can then be analyzed for efficiency of fit to a PPAR LBD binding site using the same computer-based approaches described in detail above.

VIII.B. Distinguishing Between PPAR Subtypes

The present invention discloses the ability to generate new synthetic ligands to distinguish between PPAR subtypes. As described herein, computer-designed ligands can be generated that distinguish between PPAR subtypes, thereby allowing the generation of either tissue specific or function specific ligands. The atomic structural coordinates disclosed in the present invention reveal structural details unique to PPARα. These structural details can be exploited when a novel ligand is designed using the methods of the present invention or other ligand design methods known in the art. The structural features that differentiate, for example, a PPARα from a PPARγ can be targeted in ligand design. Thus, for example, a ligand can be designed that will recognize PPARα, while not interacting with other PPARs or even with moieties having similar structural features. Prior to the disclosure of the present invention, the ability to target a PPAR subtype was unattainable.

The present invention also pertains to a method for designing an agonist or modulator with desired levels of activity on the three subtypes, PPARα, PPARγ and PPARδ. In a preferred embodiment, the method comprises obtaining atomic coordinates for structures of the PPARα, PPARγ and/or PPARδ ligand binding domains. The structures can comprise PPARα, PPARγ and PPARδ each bound to various different ligands, and also can comprise structures where no ligand is present. The structures can also comprise models where a compound has been docked into a particular PPAR using a molecular docking procedure, such as the MVP program disclosed herein. Optionally, the structures comprise rotated and translated so as to superimpose corresponding Cα or backbone atoms; this facilitates the comparison of structures.

The PPARα, PPARγ and PPARδ structures can also be compared using a computer graphics system to identify regions of the ligand binding site

that have similar shape and electrostatic character, and to identify regions of the ligand binding site that are narrowed or constricted in one or two of the PPARs compared with the other(s). Since these three PPARs are subject to conformational changes, attention is paid to the range of motion observed for each protein atom over the whole collection of structures. The ligand structures, including both those determined by X-ray crystallography and those modeled using molecular docking procedures, can be examined using a computer graphics system to identify ligands where a chemical modification could increase or decrease binding to a particular PPAR, or decrease activity against a particular PPAR. Additionally or alternatively, the chemical modification can introduce a group into a volume that is normally occupied by an atom of that PPAR.

Optionally, to selectively decrease activity against a particular PPAR, the chemical modification can be made so as to occupy volume that is normally occupied by atoms of that particular PPAR, but not by atoms of the other PPARs. To increase activity against a particular PPAR, a chemical modification can be made that improves interactions with that particular PPAR. To selectively increase activity against a particular PPAR, a chemical modification can be made that improves the interactions with that particular PPAR, but does not improve the interactions with the other PPARs. Other design principles can also be used to increase or decrease activity on a particular PPAR.

Thus, various possible compounds and chemical modfications can be considered and compared graphically, and with molecular modeling tools, for synthetic feasibility and likelihood of achieving the desired profile of activation of PPARα, PPARγ and PPARδ. Compounds that appear synthetically feasible and that have a good likelihood of achieving the desired profile are synthesized. The compounds can then be tested for binding and/or activation of PPARα, PPARγ and PPARδ, and tested for their overall biological effect.

VIII.C. Method of Screening for Chemical and Biological Modulators of the Biological Activity of PPARα

A candidate substance identified according to a screening assay of the present invention has an ability to modulate the biological activity of a PPAR or a PPAR LBD polypeptide. In a preferred embodiment, such a candidate compound can have utility in the treatment of disorders and conditions associated with the biological activity of a PPARα or a PPARα LBD polypeptide, including lipid homeostasis.

In a cell-free system, the method comprises the steps of establishing a control system comprising a crystalline PPARα polypeptide and a ligand which is capable of binding to the polypeptide; establishing a test system comprising a crystalline PPARα polypeptide, the ligand, and a candidate compound; and determining whether the candidate compound modulates the activity of the polypeptide by comparison of the test and control systems. A representative ligand comprises Compound 1 or other small molecule; and in this embodiment, the biological activity or property screened includes binding affinity.

In another embodiment of the invention, a crystalline form of a PPARα polypeptide or a catalytic or immunogenic fragment or oligopeptide thereof, can be used for screening libraries of compounds in any of a variety of drug screening techniques. The fragment employed in such a screening can be affixed to a solid support. The formation of binding complexes, between a crystalline PPARα polypeptide and the agent being tested, will be detected. In a preferred embodiment, the crystalline PPARα polypeptide has an amino acid sequence of SEQ ID NO:2. When a PPARα LBD polypeptide is employed, a preferred embodiment will include a crystalline PPARα polypeptide having the amino acid sequence of SEQ ID NO:4.

Another technique for drug screening which can be used provides for high throughput screening of compounds having suitable binding affinity to the protein of interest as described in published PCT application WO 84/03564, herein incorporated by reference. In this method, as applied to a crystalline

polypeptide of the present invention, large numbers of different small test compounds are synthesized on a solid substrate, such as plastic pins or some other surface. The test compounds are reacted with the crystalline polypeptide, or fragments thereof. Bound polypeptide is then detected by methods well known to those of skill in the art. The crystalline polypeptide can also be placed directly onto plates for use in the aforementioned drug screening techniques.

In yet another embodiment, a method of screening for a modulator of a PPARα or a PPARα LBD polypeptide comprises: providing a library of test samples; contacting a crystalline form of PPARα or a crystalline form of an PPARα LBD polypeptide with each test sample; detecting an interaction between a test sample and a crystalline form of a PPARα or a crystalline form of a PPARα LBD polypeptide; identifying a test sample that interacts with a crystalline form of a PPARα or a crystalline form of a PPARα LBD polypeptide; and isolating a test sample that interacts with a crystalline form of a PPARα or a crystalline form of a PPARα LBD polypeptide.

In each of the foregoing embodiments, an interaction can be detected spectrophotometrically, radiologically or immunologically. An interaction between a crystalline form of a PPARα or a crystalline form of a PPARα LBD polypeptide and a test sample can also be quantified using methodology known to those of skill in the art.

In accordance with the present invention there is also provided a rapid and high throughput screening method that relies on the methods described above. This screening method comprises separately contacting each of a plurality of substantially identical samples with crystalline form of a PPARα or a crystalline form of a PPARα LBD and detecting a resulting binding complex. In such a screening method the plurality of samples preferably comprises more than about 10^4 samples, or more preferably comprises more than about 5×10^4 samples.

VIII.D. Method of Identifying Compounds Which Inhibit Ligand Binding

In one aspect of the present invention, an assay method for identifying a compound that inhibits binding of a ligand to a PPAR polypeptide is disclosed. A ligand of PPARα, such as Compound 1, can be used in the assay method as the ligand against which the inhibition by a test compound is gauged. The method comprises (a) incubating a PPAR polypeptide with a ligand in the presence of a test inhibitor compound; (b) determining an amount of ligand that is bound to the PPAR polypeptide, wherein decreased binding of ligand to the PPAR polypeptide in the presence of the test inhibitor compound relative to binding in the absence of the test inhibitor compound is indicative of inhibition; and (c) identifying the test compound as an inhibitor of ligand binding if decreased ligand binding is observed. Preferably, the ligand is Compound 1.

In another aspect of the present invention, the disclosed assay method can be used in the structural refinement of candidate PPAR inhibitors. For example, multiple rounds of optimization can be followed by gradual structural changes in a strategy of inhibitor design. A strategy such as this is made possible by the disclosure of the coordinates of the PPARα LBD.

IX. Design, Preparation and Structural Analysis of Additional PPARα and PPARα LBD Mutants and Structural Equivalents

The present invention provides for the generation of PPAR and PPAR mutants (preferably PPARα and PPARα LBD mutants), and the ability to solve the crystal structures of those that crystallize. More particularly, through the provision of the three-dimensional structure of a PPARα LBD, desirable sites for mutation can be identified.

The structure coordinates of a PPARα LBD provided in accordance with the present invention also facilitate the identification of related proteins or enzymes analogous to PPARα in function, structure or both, (for example, a PPARγ) which can lead to novel therapeutic modes for treating or preventing a range of disease states.

IX.A. Sterically Similar Compounds

A further aspect of the present invention is that sterically similar compounds can be formulated to mimic the key portions of a PPAR LBD structure. Such compounds are functional equivalents. The generation of a structural functional equivalent can be achieved by the techniques of modeling and chemical design known to those of skill in the art and described herein. Modeling and chemical design of PPAR and PPAR LBD structural equivalents can be based on the structure coordinates of a crystalline PPARα LBD polypeptide of the present invention. It will be understood that all such sterically similar constructs fall within the scope of the present invention.

IX.B. PPARα Polypeptides

The generation of chimeric PPAR polypeptides is also an aspect of the present invention. Such a chimeric polypeptide can comprise a PPAR LBD polypeptide or a portion of a PPAR LBD, (e.g. a PPARα LBD) that is fused to a candidate polypeptide or a suitable region of the candidate polypeptide, for example PPARγ. Throughout the present disclosure it is intended that the term "mutant" encompass not only mutants of a PPAR LBD polypeptide but chimeric proteins generated using a PPAR LBD as well. It is thus intended that the following discussion of mutant PPAR LBDs apply *mutatis mutandis* to chimeric PPAR and PPAR LBD polypeptides and to structural equivalents thereof.

In accordance with the present invention, a mutation can be directed to a particular site or combination of sites of a wild-type PPAR LBD. For example, an accessory binding site or the binding pocket can be chosen for mutagenesis. Similarly, a residue having a location on, at or near the surface of the polypeptide can be replaced, resulting in an altered surface charge of one or more charge units, as compared to the wild-type PPAR and PPAR LBD. Alternatively, an amino acid residue in a PPAR or a PPAR LBD can be chosen for replacement based on its hydrophilic or hydrophobic characteristics.

Such mutants can be characterized by any one of several different properties as compared with the wild-type PPAR LBD. For example, such mutants can have an altered surface charge of one or more charge units, or can have an increase in overall stability. Other mutants can have altered substrate specificity in comparison with, or a higher specific activity than, a wild-type PPAR or PPAR LBD.

PPAR and PPAR LBD mutants of the present invention can be generated in a number of ways. For example, the wild-type sequence of a PPAR or a PPAR LBD can be mutated at those sites identified using this invention as desirable for mutation, by means of oligonucleotide-directed mutagenesis or other conventional methods, such as deletion. Alternatively, mutants of a PPAR or a PPAR LBD can be generated by the site-specific replacement of a particular amino acid with an unnaturally occurring amino acid. In addition, PPAR or PPAR LBD mutants can be generated through replacement of an amino acid residue, for example, a particular cysteine or methionine residue, with selenocysteine or selenomethionine. This can be achieved by growing a host organism capable of expressing either the wild-type or mutant polypeptide on a growth medium depleted of either natural cysteine or methionine (or both) but enriched in selenocysteine or selenomethionine (or both).

Mutations can be introduced into a DNA sequence coding for a PPAR or a PPAR LBD using synthetic oligonucleotides. These oligonucleotides contain nucleotide sequences flanking the desired mutation sites. Mutations can be generated in the full-length DNA sequence of a PPAR or a PPAR LBD or in any sequence coding for polypeptide fragments of a PPAR or a PPAR LBD.

According to the present invention, a mutated PPAR or PPAR LBD DNA sequence produced by the methods described above, or any alternative methods known in the art, can be expressed using an expression vector. An expression vector, as is well known to those of skill in the art, typically includes elements that permit autonomous replication in a host cell independent of the host genome, and one or more phenotypic markers for

selection purposes. Either prior to or after insertion of the DNA sequences surrounding the desired PPAR or PPAR LBD mutant coding sequence, an expression vector also will include control sequences encoding a promoter, operator, ribosome binding site, translation initiation signal, and, optionally, a repressor gene or various activator genes and a signal for termination. In some embodiments, where secretion of the produced mutant is desired, nucleotides encoding a "signal sequence" can be inserted prior to a PPAR or a PPAR LBD mutant coding sequence. For expression under the direction of the control sequences, a desired DNA sequence must be operatively linked to the control sequences; that is, the sequence must have an appropriate start signal in front of the DNA sequence encoding the PPAR or PPAR LBD mutant, and the correct reading frame to permit expression of that sequence under the control of the control sequences and production of the desired product encoded by that PPAR or PPAR LBD sequence must be maintained.

Any of a wide variety of well-known available expression vectors can be useful to express a mutated PPAR or PPAR LBD coding sequences of this invention. These include for example, vectors consisting of segments of chromosomal, non-chromosomal and synthetic DNA sequences, such as various known derivatives of SV40, known bacterial plasmids, e.g., plasmids from *E. coli* including col E1, pCR1, pBR322, pMB9 and their derivatives, wider host range plasmids, e.g., RP4, phage DNAs, e.g., the numerous derivatives of phage λ, e.g., NM 989, and other DNA phages, e.g., M13 and filamentous single stranded DNA phages, yeast plasmids and vectors derived from combinations of plasmids and phage DNAs, such as plasmids which have been modified to employ phage DNA or other expression control sequences. In the preferred embodiments of this invention, vectors amenable to expression in a pRSETA-based expression system are employed. The pRSETA expression system is available from Invitrogen, Inc., Carlsbad, California.

In addition, any of a wide variety of expression control sequences—sequences that control the expression of a DNA sequence when operatively linked to it—can be used in these vectors to express the mutated DNA

sequences according to this invention. Such useful expression control sequences, include, for example, the early and late promoters of SV40 for animal cells, the lac system, the trp system the TAC or TRC system, the major operator and promoter regions of phage λ, the control regions of fd coat protein, all for *E. coli*, the promoter for 3-phosphoglycerate kinase or other glycolytic enzymes, the promoters of acid phosphatase, e.g., Pho5, the promoters of the yeast α-mating factors for yeast, and other sequences known to control the expression of genes of prokaryotic or eukaryotic cells or their viruses, and various combinations thereof.

A wide variety of hosts are also useful for producing mutated PPARα and PPARα LBD polypeptides according to this invention. These hosts include, for example, bacteria, such as *E. coli*, *Bacillus* and *Streptomyces*, fungi, such as yeasts, and animal cells, such as CHO and COS-1 cells, plant cells, insect cells, such as Sf9 cells, and transgenic host cells.

It should be understood that not all expression vectors and expression systems function in the same way to express mutated DNA sequences of this invention, and to produce modified PPAR and PPAR LBD polypeptides or PPAR or PPAR LBD mutants. Neither do all hosts function equally well with the same expression system. One of skill in the art can, however, make a selection among these vectors, expression control sequences and hosts without undue experimentation and without departing from the scope of this invention. For example, an important consideration in selecting a vector will be the ability of the vector to replicate in a given host. The copy number of the vector, the ability to control that copy number, and the expression of any other proteins encoded by the vector, such as antibiotic markers, should also be considered.

In selecting an expression control sequence, a variety of factors should also be considered. These include, for example, the relative strength of the system, its controllability and its compatibility with the DNA sequence encoding a modified PPAR or PPAR LBD polypeptide of this invention, with

particular regard to the formation of potential secondary and tertiary structures.

Hosts should be selected by consideration of their compatibility with the chosen vector, the toxicity of a modified PPAR or PPAR LBD to them, their ability to express mature products, their ability to fold proteins correctly, their fermentation requirements, the ease of purification of a modified PPAR or PPAR LBD and safety. Within these parameters, one of skill in the art can select various vector/expression control system/host combinations that will produce useful amounts of a mutant PPAR or PPAR LBD. A mutant PPAR or PPAR LBD produced in these systems can be purified by a variety of conventional steps and strategies, including those used to purify the wild-type PPAR or PPAR LBD.

Once a PPAR LBD mutation(s) has been generated in the desired location, such as an active site or dimerization site, the mutants can be tested for any one of several properties of interest. For example, mutants can be screened for an altered charge at physiological pH. This is determined by measuring the mutant PPAR or PPAR LBD isoelectric point (pI) and comparing the observed value with that of the wild-type parent. Isoelectric point can be measured by gel-electrophoresis according to the method of Wellner (Wellner, (1971) *Anal. Chem.* 43: 597). A mutant PPAR or PPAR LBD polypeptide containing a replacement amino acid located at the surface of the enzyme, as provided by the structural information of this invention, can lead to an altered surface charge and an altered pI.

IX.C. Generation of an Engineered PPARα LBD or PPARα LBD Mutant

In another aspect of the present invention, a unique PPAR or PPAR LBD polypeptide can be generated. Such a mutant can facilitate purification and the study of the ligand-binding abilities of a PPAR polypeptide.

As used in the following discussion, the terms "engineered PPAR", "engineered PPAR LDB", "PPAR mutant", and "PPAR LBD mutant" refers to polypeptides having amino acid sequences which contain at least one

mutation in the wild-type sequence. The terms also refer to PPAR and PPAR LBD polypeptides which are capable of exerting a biological effect in that they comprise all or a part of the amino acid sequence of an engineered PPAR or PPAR LBD mutant polypeptide of the present invention, or cross-react with antibodies raised against an engineered PPAR or PPAR LBD mutant polypeptide, or retain all or some or an enhanced degree of the biological activity of the engineered PPAR or PPAR LBD mutant amino acid sequence or protein. Such biological activity can include the binding of small molecules in general, and the binding of Compound 1 in particular.

The terms "engineered PPAR LBD" and "PPAR LBD mutant" also includes analogs of an engineered PPAR LBD or PPAR LBD mutant polypeptide. By "analog" is intended that a DNA or polypeptide sequence can contain alterations relative to the sequences disclosed herein, yet retain all or some or an enhanced degree of the biological activity of those sequences. Analogs can be derived from genomic nucleotide sequences or from other organisms, or can be created synthetically. Those of skill in the art will appreciate that other analogs, as yet undisclosed or undiscovered, can be used to design and/or construct PPAR LBD or PPAR LBD mutant analogs. There is no need for an engineered PPAR LBD or PPAR LBD mutant polypeptide to comprise all or substantially all of the amino acid sequence of SEQ ID NOs:2 or 4. Shorter or longer sequences are anticipated to be of use in the invention; shorter sequences are herein referred to as "segments". Thus, the terms "engineered PPAR LBD" and "PPAR LBD mutant" also includes fusion, chimeric or recombinant engineered PPAR LBD or PPAR LBD mutant polypeptides and proteins comprising sequences of the present invention. Methods of preparing such proteins are disclosed herein above and are known in the art.

IX.D. Sequence Similarity and Identity

As used herein, the term "substantially similar" means that a particular sequence varies from nucleic acid sequence of SEQ ID NOs:1 or 3, or the amino acid sequence of SEQ ID NOs:2 or 4 by one or more deletions,

substitutions, or additions, the net effect of which is to retain at least some of biological activity of the natural gene, gene product, or sequence. Such sequences include "mutant" or "polymorphic" sequences, or sequences in which the biological activity and/or the physical properties are altered to some degree but retains at least some or an enhanced degree of the original biological activity and/or physical properties. In determining nucleic acid sequences, all subject nucleic acid sequences capable of encoding substantially similar amino acid sequences are considered to be substantially similar to a reference nucleic acid sequence, regardless of differences in codon sequences or substitution of equivalent amino acids to create biologically functional equivalents.

IX.D.1. Sequences That are Substantially Identical to an Engineered PPAR or PPAR LBD Mutant Sequence of the Present Invention

Nucleic acids that are substantially identical to a nucleic acid sequence of an engineered PPAR or PPAR LBD mutant of the present invention, e.g. allelic variants, genetically altered versions of the gene, etc., bind to an engineered PPAR or PPAR LBD mutant sequence under stringent hybridization conditions. By using probes, particularly labeled probes of DNA sequences, one can isolate homologous or related genes. The source of homologous genes can be any species, e.g. primate species; rodents, such as rats and mice, canines, felines, bovines, equines, yeast, nematodes, etc.

Between mammalian species, e.g. human and mouse, homologs have substantial sequence similarity, i.e. at least 75% sequence identity between nucleotide sequences. Sequence similarity is calculated based on a reference sequence, which can be a subset of a larger sequence, such as a conserved motif, coding region, flanking region, etc. A reference sequence will usually be at least about 18 nt long, more usually at least about 30 nt long, and can extend to the complete sequence that is being compared. Algorithms for sequence analysis are known in the art, such as BLAST, described in Altschul et al., (1990) *J. Mol. Biol.* 215: 403-10.

Percent identity or percent similarity of a DNA or peptide sequence can be determined, for example, by comparing sequence information using the GAP computer program, available from the University of Wisconsin Geneticist Computer Group. The GAP program utilizes the alignment method of Needleman et al., (1970) *J. Mol. Biol.* 48: 443, as revised by Smith et al., (1981) *Adv. Appl. Math.* 2:482. Briefly, the GAP program defines similarity as the number of aligned symbols (i.e., nucleotides or amino acids) which are similar, divided by the total number of symbols in the shorter of the two sequences. The preferred parameters for the GAP program are the default parameters, which do not impose a penalty for end gaps. See, e.g., Schwartz et al., eds., (1979), Atlas of Protein Sequence and Structure, National Biomedical Research Foundation, pp. 357-358, and Gribskov et al., (1986) *Nucl. Acids. Res.* 14: 6745.

The term "similarity" is contrasted with the term "identity". Similarity is defined as above; "identity", however, means a nucleic acid or amino acid sequence having the same amino acid at the same relative position in a given family member of a gene family. Homology and similarity are generally viewed as broader terms than the term identity. Biochemically similar amino acids, for example leucine/isoleucine or glutamate/aspartate, can be present at the same position—these are not identical per se, but are biochemically "similar." As disclosed herein, these are referred to as conservative differences or conservative substitutions. This differs from a conservative mutation at the DNA level, which changes the nucleotide sequence without making a change in the encoded amino acid, e.g. TCC to TCA, both of which encode serine.

As used herein, DNA analog sequences are "substantially identical" to specific DNA sequences disclosed herein if: (a) the DNA analog sequence is derived from coding regions of the nucleic acid sequence shown in SEQ ID NOs:1 or 3; or (b) the DNA analog sequence is capable of hybridization with DNA sequences of (a) under stringent conditions and which encode a biologically active PPARα or PPARα LBD gene product; or (c) the DNA sequences are degenerate as a result of alternative genetic code to the DNA

analog sequences defined in (a) and/or (b). Substantially identical analog proteins and nucleic acids will have between about 70% and 80%, preferably between about 81% to about 90% or even more preferably between about 91% and 99% sequence identity with the corresponding sequence of the native protein or nucleic acid. Sequences having lesser degrees of identity but comparable biological activity are considered to be equivalents.

As used herein, "stringent conditions" means conditions of high stringency, for example 6XSSC, 0.2% polyvinylpyrrolidone, 0.2% Ficoll, 0.2% bovine serum albumin, 0.1% sodium dodecyl sulfate, 100 µg/ml salmon sperm DNA and 15% formamide at 68°C. For the purposes of specifying additional conditions of high stringency, preferred conditions are salt concentration of about 200 mM and temperature of about 45°C. One example of such stringent conditions is hybridization at 4XSSC, at 65°C, followed by a washing in 0.1XSSC at 65°C for one hour. Another exemplary stringent hybridization scheme uses 50% formamide, 4XSSC at 42°C.

In contrast, nucleic acids having sequence similarity are detected by hybridization under lower stringency conditions. Thus, sequence identity can be determined by hybridization under lower stringency conditions, for example, at 50°C or higher and 0.1XSSC (9 mM NaCl/0.9 mM sodium citrate) and the sequences will remain bound when subjected to washing at 55°C in 1XSSC.

IX.D.2. Complementarity and Hybridization to an Engineered PPARα or PPARα LBD Mutant Sequence

As used herein, the term "complementary sequences" means nucleic acid sequences which are base-paired according to the standard Watson-Crick complementarity rules. The present invention also encompasses the use of nucleotide segments that are complementary to the sequences of the present invention.

Hybridization can also be used for assessing complementary sequences and/or isolating complementary nucleotide sequences. As discussed above, nucleic acid hybridization will be affected by such conditions

as salt concentration, temperature, or organic solvents, in addition to the base composition, length of the complementary strands, and the number of nucleotide base mismatches between the hybridizing nucleic acids, as will be readily appreciated by those skilled in the art. Stringent temperature conditions will generally include temperatures in excess of about 30°C, typically in excess of about 37°C, and preferably in excess of about 45°C. Stringent salt conditions will ordinarily be less than about 1,000 mM, typically less than about 500 mM, and preferably less than about 200 mM. However, the combination of parameters is much more important than the measure of any single parameter. See, e.g., Wetmur & Davidson, (1968) *J. Mol. Biol.* 31: 349-70. Determining appropriate hybridization conditions to identify and/or isolate sequences containing high levels of homology is well known in the art. See, e.g., Sambrook et al., (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor, New York.

IX.D.3. Functional Equivalents of an Engineered PPARα or PPARα LBD Mutant Nucleic Acid Sequence of the Present Invention

As used herein, the term "functionally equivalent codon" is used to refer to codons that encode the same amino acid, such as the ACG and AGU codons for serine. PPARα or PPARα LBD-encoding nucleic acid sequences comprising SEQ ID NOs:1 and 3 which have functionally equivalent codons are covered by the present invention. Thus, when referring to the sequence example presented in SEQ ID NOs:1 and 3, applicants contemplate substitution of functionally equivalent codons into the sequence example of SEQ ID NOs:1 and 3. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

It will also be understood by those of skill in the art that amino acid and nucleic acid sequences can include additional residues, such as additional N- or C-terminal amino acids or 5' or 3' nucleic acid sequences, and yet still be essentially as set forth in one of the sequences disclosed herein, so long as the sequence retains biological protein activity where polypeptide expression

is concerned. The addition of terminal sequences particularly applies to nucleic acid sequences which can, for example, include various non-coding sequences flanking either of the 5' or 3' portions of the coding region or can include various internal sequences, i.e., introns, which are known to occur within genes.

IX.D.4. Biological Equivalents

The present invention envisions and includes biological equivalents of a engineered PPAR or PPAR LBD mutant polypeptide of the present invention. The term "biological equivalent" refers to proteins having amino acid sequences which are substantially identical to the amino acid sequence of an engineered PPAR LBD mutant of the present invention and which are capable of exerting a biological effect in that they are capable of binding small molecules or cross-reacting with anti- PPAR or PPAR LBD mutant antibodies raised against an engineered mutant PPAR or PPAR LBD polypeptide of the present invention.

For example, certain amino acids can be substituted for other amino acids in a protein structure without appreciable loss of interactive capacity with, for example, structures in the nucleus of a cell. Since it is the interactive capacity and nature of a protein that defines that protein's biological functional activity, certain amino acid sequence substitutions can be made in a protein sequence (or the nucleic acid sequence encoding it) to obtain a protein with the same, enhanced, or antagonistic properties. Such properties can be achieved by interaction with the normal targets of the protein, but this need not be the case, and the biological activity of the invention is not limited to a particular mechanism of action. It is thus in accordance with the present invention that various changes can be made in the amino acid sequence of an engineered PPAR or PPAR LBD mutant polypeptide of the present invention or its underlying nucleic acid sequence without appreciable loss of biological utility or activity.

Biologically equivalent polypeptides, as used herein, are polypeptides in which certain, but not most or all, of the amino acids can be substituted.

Thus, when referring to the sequence examples presented in SEQ ID NOs:1 and 3, applicants envision substitution of codons that encode biologically equivalent amino acids, as described herein, into the sequence example of SEQ ID NOs:2 and 4, respectively. Thus, applicants are in possession of amino acid and nucleic acids sequences which include such substitutions but which are not set forth herein in their entirety for convenience.

Alternatively, functionally equivalent proteins or peptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged, e.g. substitution of Ile for Leu. Changes designed by man can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test an engineered PPAR or PPAR LBD mutant polypeptide of the present invention in order to modulate lipid-binding or other activity, at the molecular level.

Amino acid substitutions, such as those which might be employed in modifying an engineered PPAR or PPAR LBD mutant polypeptide of the present invention are generally, but not necessarily, based on the relative similarity of the amino acid side-chain substituents, for example, their hydrophobicity, hydrophilicity, charge, size, and the like. An analysis of the size, shape and type of the amino acid side-chain substituents reveals that arginine, lysine and histidine are all positively charged residues; that alanine, glycine and serine are all of similar size; and that phenylalanine, tryptophan and tyrosine all have a generally similar shape. Therefore, based upon these considerations, arginine, lysine and histidine; alanine, glycine and serine; and phenylalanine, tryptophan and tyrosine; are defined herein as biologically functional equivalents. Other biologically functionally equivalent changes will be appreciated by those of skill in the art. It is implicit in the above discussion, however, that one of skill in the art can appreciate that a radical, rather than a conservative substitution is warranted in a given situation. Non-conservative substitutions in engineered mutant PPAR or PPAR LBD polypeptides of the present invention are also an aspect of the present invention.

In making biologically functional equivalent amino acid substitutions, the hydropathic index of amino acids can be considered. Each amino acid has been assigned a hydropathic index on the basis of their hydrophobicity and charge characteristics, these are: isoleucine (+ 4.5); valine (+ 4.2); leucine (+ 3.8); phenylalanine (+ 2.8); cysteine (+ 2.5); methionine (+ 1.9); alanine (+ 1.8); glycine (-0.4); threonine (-0.7); serine (-0.8); tryptophan (-0.9); tyrosine (-1.3); proline (-1.6); histidine (-3.2); glutamate (-3.5); glutamine (-3.5); aspartate (-3.5); asparagine (-3.5); lysine (-3.9); and arginine (-4.5).

The importance of the hydropathic amino acid index in conferring interactive biological function on a protein is generally understood in the art (Kyte & Doolittle, (1982), *J. Mol. Biol.* 157: 105-132, incorporated herein by reference). It is known that certain amino acids can be substituted for other amino acids having a similar hydropathic index or score and still retain a similar biological activity. In making changes based upon the hydropathic index, the substitution of amino acids whose hydropathic indices are within ±2 of the original value is preferred, those which are within ±1 of the original value are particularly preferred, and those within ±0.5 of the original value are even more particularly preferred.

It is also understood in the art that the substitution of like amino acids can be made effectively on the basis of hydrophilicity. U.S. Patent No. 4,554,101, incorporated herein by reference, states that the greatest local average hydrophilicity of a protein, as governed by the hydrophilicity of its adjacent amino acids, correlates with its immunogenicity and antigenicity, i.e. with a biological property of the protein. It is understood that an amino acid can be substituted for another having a similar hydrophilicity value and still obtain a biologically equivalent protein.

As detailed in U.S. Patent No. 4,554,101, the following hydrophilicity values have been assigned to amino acid residues: arginine (+ 3.0); lysine (+ 3.0); aspartate (+ 3.0±1); glutamate (+ 3.0±1); serine (+ 0.3); asparagine (+ 0.2); glutamine (+ 0.2); glycine (0); threonine (-0.4); proline (-0.5±1); alanine (-0.5); histidine (-0.5); cysteine (-1.0); methionine (-1.3); valine (-1.5); leucine (-1.8); isoleucine (-1.8); tyrosine (-2.3); phenylalanine (-2.5); tryptophan (-3.4).

In making changes based upon similar hydrophilicity values, the substitution of amino acids whose hydrophilicity values are within ±2 of the original value is preferred, those which are within ±1 of the original value are particularly preferred, and those within ±0.5 of the original value are even more particularly preferred.

While discussion has focused on functionally equivalent polypeptides arising from amino acid changes, it will be appreciated that these changes can be effected by alteration of the encoding DNA, taking into consideration also that the genetic code is degenerate and that two or more codons can code for the same amino acid.

Thus, it will also be understood that this invention is not limited to the particular amino acid and nucleic acid sequences of SEQ ID NOs:1-4. Recombinant vectors and isolated DNA segments can therefore variously include an engineered PPARα or PPARα LBD mutant polypeptide-encoding region itself, include coding regions bearing selected alterations or modifications in the basic coding region, or include larger polypeptides which nevertheless comprise an PPARα or PPARα LBD mutant polypeptide-encoding regions or can encode biologically functional equivalent proteins or polypeptides which have variant amino acid sequences. Biological activity of an engineered PPARα or PPARα LBD mutant polypeptide can be determined, for example, by lipid-binding assays known to those of skill in the art.

The nucleic acid segments of the present invention, regardless of the length of the coding sequence itself, can be combined with other DNA sequences, such as promoters, enhancers, polyadenylation signals, additional restriction enzyme sites, multiple cloning sites, other coding segments, and the like, such that their overall length can vary considerably. It is therefore contemplated that a nucleic acid fragment of almost any length can be employed, with the total length preferably being limited by the ease of preparation and use in the intended recombinant DNA protocol. For example, nucleic acid fragments can be prepared which include a short stretch complementary to a nucleic acid sequence set forth in SEQ ID NOs:1 and 3,

such as about 10 nucleotides, and which are up to 10,000 or 5,000 base pairs in length. DNA segments with total lengths of about 4,000, 3,000, 2,000, 1,000, 500, 200, 100, and about 50 base pairs in length are also useful.

The DNA segments of the present invention encompass biologically functional equivalents of engineered PPAR or PPAR LBD mutant polypeptides. Such sequences can rise as a consequence of codon redundancy and functional equivalency that are known to occur naturally within nucleic acid sequences and the proteins thus encoded. Alternatively, functionally equivalent proteins or polypeptides can be created via the application of recombinant DNA technology, in which changes in the protein structure can be engineered, based on considerations of the properties of the amino acids being exchanged. Changes can be introduced through the application of site-directed mutagenesis techniques, e.g., to introduce improvements to the antigenicity of the protein or to test variants of an engineered PPAR or PPAR LBD mutant of the present invention in order to examine the degree of lipid-binding activity, or other activity at the molecular level. Various site-directed mutagenesis techniques are known to those of skill in the art and can be employed in the present invention.

The invention further encompasses fusion proteins and peptides wherein an engineered PPAR or PPAR LBD mutant coding region of the present invention is aligned within the same expression unit with other proteins or peptides having desired functions, such as for purification or immunodetection purposes.

Recombinant vectors form important further aspects of the present invention. Particularly useful vectors are those in which the coding portion of the DNA segment is positioned under the control of a promoter. The promoter can be that naturally associated with a PPAR gene, as can be obtained by isolating the 5' non-coding sequences located upstream of the coding segment or exon, for example, using recombinant cloning and/or PCR technology and/or other methods known in the art, in conjunction with the compositions disclosed herein.

In other embodiments, certain advantages will be gained by positioning the coding DNA segment under the control of a recombinant, or heterologous, promoter. As used herein, a recombinant or heterologous promoter is a promoter that is not normally associated with a PPAR gene in its natural environment. Such promoters can include promoters isolated from bacterial, viral, eukaryotic, or mammalian cells. Naturally, it will be important to employ a promoter that effectively directs the expression of the DNA segment in the cell type chosen for expression. The use of promoter and cell type combinations for protein expression is generally known to those of skill in the art of molecular biology (See, e.g., Sambrook et al., (1989) Molecular Cloning: A Laboratory Manual, Cold Spring Harbor Laboratory, New York, specifically incorporated herein by reference). The promoters employed can be constitutive or inducible and can be used under the appropriate conditions to direct high level expression of the introduced DNA segment, such as is advantageous in the large-scale production of recombinant proteins or peptides. One preferred promoter system contemplated for use in high-level expression is a T7 promoter-based system.

X. The Role of the Three-Dimensional Structure of the PPARα LDB in Solving Additional PPAR Crystals

Because polypeptides can crystallize in more than one crystal form, the structural coordinates of a PPARα LBD, or portions thereof, as provided by the present invention, are particularly useful in solving the structure of other crystal forms of PPARα and the crystalline forms of other PPARs. The coordinates provided in the present invention can also be used to solve the structure of PPAR or PPAR LBD mutants (such as those described in Section IX above), PPAR LDB co-complexes, or of the crystalline form of any other protein with significant amino acid sequence homology to any functional domain of PPAR.

X.A. Determining the Three-Dimensional Structure of a Polypeptide Using the Three-Dimensional Structure of the PPARα LBD as a Template in Molecular Replacement

One method that can be employed for the purpose of solving additional PPAR crystal structures is molecular replacement. See generally, Rossmann, ed, (1972) The Molecular Replacement Method, Gordon & Breach, New York. In the molecular replacement method, the unknown crystal structure, whether it is another crystal form of a PPARα or a PPARα LBD, (i.e. a PPARα or a PPARα LBD mutant), or a PPARα or a PPARα LBD polypeptide complexed with another compound (a "co-complex"), or the crystal of some other protein with significant amino acid sequence homology to any functional region of the PPARα LBD, can be determined using the PPARα LBD structure coordinates provided in Table 2. This method provides an accurate structural form for the unknown crystal more quickly and efficiently than attempting to determine such information *ab initio*.

In addition, in accordance with this invention, PPARα or PPARα LBD mutants can be crystallized in complex with known modulators. The crystal structures of a series of such complexes can then be solved by molecular replacement and compared with that of wild-type PPARα or the wild-type PPARα LBD. Potential sites for modification within the various binding sites of the enzyme can thus be identified. This information provides an additional tool for determining the most efficient binding interactions, for example, increased hydrophobic interactions, between the PPARα LBD and a chemical entity or compound.

All of the complexes referred to in the present disclosure can be studied using X-ray diffraction techniques (See, e.g., Blundell & Johnson (1985) *Method.Enzymol.*, 114A & 115B, (Wyckoff et al., eds.), Academic Press) and can be refined using computer software, such as the X-PLOR™ program (Brünger, (1992) *X-PLOR, Version 3.1. A System for X-ray Crystallography and NMR*, Yale University Press, New Haven, Connecticut; X-PLOR is available from Molecular Simulations, Inc., San Diego, California).

This information can thus be used to optimize known classes of PPAR and PPAR LBD modulators, and more importantly, to design and synthesize novel classes of PPAR and PPAR LBD modulators.

Laboratory Examples

The following Laboratory Examples have been included to illustrate preferred modes of the invention. Certain aspects of the following Laboratory Examples are described in terms of techniques and procedures found or contemplated by the present inventors to work well in the practice of the invention. These Laboratory Examples are exemplified through the use of standard laboratory practices of the inventors. In light of the present disclosure and the general level of skill in the art, those of skill will appreciate that the following Laboratory Examples are intended to be exemplary only and that numerous changes, modifications and alterations can be employed without departing from the spirit and scope of the invention.

Laboratory Example 1

Protein Preparation

The nucleic acid sequence encoding the PPARα ligand binding domain (amino acids 192-468) tagged with MKKGHHHHHHG (SEQ ID NO: 9) was operatively linked to and expressed using the T7 promoter of plasmid vector pRSETA. BL21(DE3) *E. coli* cells transformed with this expression vector were grown at 24°C in shaker flasks for 66 hours on 2xYT medium (16 g/L Bacto-Tryptone, 10 g/L yeast extract, 5 g/L NaCl, QC with distilled water) with 50 mg/L carbenicillin to an OD_{600} of approximately 9.0. The cells were harvested, resuspended with 20 ml extract Buffer (20 mM HEPES, pH 7.5, 50 mM imidozle, 250 mM NaCl and a pinch of lysozyme) per liter of cells and were lysed by sonication for 20 minutes on ice. The lysed cells were centrifuged at 40,000g for 40 minutes and the supernatant was loaded on a 100 ml Ni-agarose column.

The column was washed with 150 ml Buffer A (10% glycerol, 20 mM HEPES pH 7.5, 25 mM imidizole) and the protein was eluted with a 450 ml

gradient of Buffer B (10% glycerol, 20 mM HEPES pH 7.5, 500 mM imidozle). The protein, which eluted at 20% Buffer B, was diluted with one volume of Buffer C (20 mM HEPES, pH 7.5, 1 mM EDTA), and loaded on an 100 ml S-Sepharose™ (Pharmacia, Peapack, New Jersey) column. The column was washed with a 100 ml Buffer C and the PPARα LBD protein was eluted with a 200 ml gradient of Buffer D (20 mM HEPES, pH 7.5, 10 mM DTT, 1 M ammonium acetate). The PPAR alpha LBD eluted from the column at 43% Buffer D. The protein yield was 9 mg/ L of cells grown and was >95% pure, as determined by SDS-PAGE analysis.

The protein was then diluted to 1 mg/ml with Buffer C such that the final buffer composition was 220 mM ammonium acetate, 20 mM HEPES pH 7.5, 1 mM EDTA and 1 mM DTT. The diluted protein was aliquoted into 9 ml aliquots, flash frozen with liquid nitrogen and stored at -80°C. To prepare complexes an individual aliquot was thawed for each compound. The peptide SRC1 (See, Xu et al., (1999) *Mol. Cell* 3: 397-403) was added in a mol ratio of 1.5 as a 2mg/ 100 µl DMSO stock. The peptide was then added in a mol ratio of 5:1 as a 2mg/100 µl DMSO stock and spun at 4K for 20 min to clarify the solution before concentrating in Centriprep™ 30 filtration units (Millipore, Bedford, Massachusetts). The solution containing the PPARα LBD-SRC1 complexes was concentrated to approximately 10 mg/ml with 80% yield. The complexes were then aliquoted in single use aliquots of 30 µl, flash frozen in liquid nitrogen and stored at -80°C.

Laboratory Example 2

Crystallization and Data Collection

The crystals disclosed in this invention were grown at room temperature using the hanging drop vapor diffusion method. The hanging drops comprised 1 µl of the above protein-ligand solutions, and were mixed with an equal volume (1 µl) of well buffer comprising 7% PEG 3350, 200 mM NaF, and 12% 2,5 hexanediol.

Before data collection, crystals were transiently mixed with well buffer that contained an additional 10% hexanediol as a cryoprotectant, and then flash frozen in liquid nitrogen.

The PPARα crystals formed in the $P2_12_12$ space group, with a=61.3 Å, b = 103.5Å, c = 49.9Å. Each asymmetry unit contained a single PPARα LBD with 45% solvent content. Crystals contained Compound 1, the PPARα LBD and SRC1 peptide, in a ratio of 1:1:1. Data were collected with a Rigaku R-Axis II (Rigaku, Tokyo, Japan) detector in house, or with a MAR CCD detector in the IMCA 17ID beam line at the Argonne National Laboratory (Argonne, Illinois), and the observed reflections were reduced, merged and scaled with DENZO™ and SCALEPACK™ in the HKL2000 package (Otwinowski, (1993) in Proceedings of the CCP4 Study Weekend: Data Collection and Processing. (Sawyer et al., eds.), pp.56-62, SERC Daresbury Laboratory, England).

Laboratory Example 3

Structure Determination and Refinement

The structure was determined by molecular replacement methods with the CCP4 AmoRe program (Collaborative Computational Project Number 4, 1994; Navaza, (1994) *Acta. Cryst.* A50: 157-163) using the structure coordinates for the PPARδ LBD (Xu et al., (1999) *Mol. Cell* 3: 397-403), residues 167-441, as the initial model (Table 3). The best fitting solution gave a correlation coefficiency of 70% and an R-factor of 33%. Model building was performed with the software program QUANTA™, and structure refinement was achieved using the CNS software program (Brünger et al., (1998) *Acta. Crystallogr.* D54: 905-921). Structure refinement involved multiple cycles of manual rebuilding. The final structure (Table 2 and Figures 1, 2, 4 and 7) includes one PPARα LBD, one SRC1 peptide and Compound 1. The statistics of the structures are summarized in Table 1.

Laboratory Example 4

Computational Analysis

Surface areas were calculated using both the Connolly MS program (Connolly, (1983) *Science* 221: 709-713) and the MVP program (Lambert, (1997) in Practical Application of Computer–Aided Drug Design, (Charifson, ed.), pp. 243-303, Marcel-Dekker, New York). The C2-symmetry axis, sequence alignments and binding site accessible waters were calculated using the software program MVP.

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U.S. Patent No. 5,872,011

U.S. Patent No. 6,008,033

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TABLE 1

PARAMETERS FOR THE CRYSTALLINE FORM OF THE LIGAND BINDING DOMAIN (RESIDUES 207-441) OF PPARα IN COMPLEX WITH COMPOUND 1

X-ray Source	Glaxo Facility	IMCA
Space Group	$P2_12_12$	$P2_12_12$
Resolution (Å)	20.0- 2.4	20.0-1.8
Unique Reflections (N)	64,772	30,147
Completeness (%)	95.2	99.4
I/σ(last shell)	25.4 (3.3)	39.5 (5.2)
R_{sym}[a] (%)	9.4	4.5
Refinement Statistics		
R factor[b] (%)(2σ)		22.9
R free[c] (%)(2σ)		26.9
R.M.S.D. Bond Lengths (Å)		0.010
R.M.S.D. Bond Angles (degrees)		1.357
Number of H_2O Molecules		396
Total Non-hydrogen Atoms		2659

r.m.s.d. is the root mean square deviation from ideal geometry.

[a] $R_{sym} = \sum | I_{avg} - I_i | / \sum I_i$

[b] $R_{factor} = \sum | F_P - F_{Pcalc} | / \sum F_p$, where F_p and F_{pcalc} are observed and calculated structure factors, respectively

[c] R_{free} is calculated from a randomly chosen 10% of reflections that have never been used in refinement, and R_{factor} is calculated for the remaining 90% of reflections.

TABLE 2

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFRACTION FROM THE LIGAND BINDING DOMAIN OF PPARα in COMPLEX WITH COUPOUND 1

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	CB	ASP	A	202	14.533	5.575	19.857	1.00	78.46
2	CG	ASP	A	202	14.270	4.099	20.079	1.00	79.53
3	OD1	ASP	A	202	13.370	3.547	19.410	1.00	80.23
4	OD2	ASP	A	202	14.963	3.492	20.921	1.00	80.14
5	C	ASP	A	202	15.243	7.375	18.274	1.00	76.33
6	O	ASP	A	202	14.377	8.174	17.918	1.00	76.50
7	N	ASP	A	202	16.101	5.066	18.013	1.00	77.36
8	CA	ASP	A	202	14.925	5.890	18.412	1.00	77.08
9	N	LEU	A	203	16.488	7.739	18.565	1.00	74.80
10	CA	LEU	A	203	16.927	9.125	18.460	1.00	72.96
11	CB	LEU	A	203	18.150	9.378	19.344	1.00	73.58
12	CG	LEU	A	203	18.821	10.740	19.132	1.00	73.64
13	CD1	LEU	A	203	18.061	11.815	19.895	1.00	73.44
14	CD2	LEU	A	203	20.265	10.680	19.597	1.00	73.65
15	C	LEU	A	203	17.304	9.418	17.019	1.00	71.55
16	O	LEU	A	203	17.251	10.561	16.574	1.00	71.54
17	N	LYS	A	204	17.694	8.379	16.292	1.00	69.51
18	CA	LYS	A	204	18.088	8.548	14.905	1.00	67.63
19	CB	LYS	A	204	18.876	7.324	14.439	1.00	68.39
20	CG	LYS	A	204	19.491	7.454	13.057	1.00	68.94
21	CD	LYS	A	204	20.927	6.946	13.047	1.00	69.41
22	CE	LYS	A	204	21.072	5.632	13.805	1.00	69.58
23	NZ	LYS	A	204	22.447	5.088	13.716	1.00	70.30
24	C	LYS	A	204	16.866	8.787	14.025	1.00	65.91
25	O	LYS	A	204	16.995	9.160	12.858	1.00	66.04
26	N	SER	A	205	15.680	8.574	14.590	1.00	62.82

27	CA	SER	A	205	14.445	8.814	13.854	1.00	59.48
28	CB	SER	A	205	13.240	8.252	14.613	1.00	59.65
29	OG	SER	A	205	12.994	8.984	15.802	1.00	59.47
30	C	SER	A	205	14.330	10.331	13.751	1.00	56.82
31	O	SER	A	205	13.495	10.861	13.016	1.00	56.27
32	N	LEU	A	206	15.186	11.015	14.510	1.00	53.62
33	CA	LEU	A	206	15.240	12.473	14.540	1.00	50.75
34	CB	LEU	A	206	16.362	12.935	15.477	1.00	50.59
35	CG	LEU	A	206	16.728	14.421	15.542	1.00	49.94
36	CD1	LEU	A	206	15.575	15.224	16.114	1.00	49.18
37	CD2	LEU	A	206	17.972	14.595	16.403	1.00	49.63
38	C	LEU	A	206	15.490	13.018	13.142	1.00	48.97
39	O	LEU	A	206	15.015	14.098	12.795	1.00	49.11
40	N	ALA	A	207	16.239	12.262	12.344	1.00	46.47
41	CA	ALA	A	207	16.555	12.671	10.983	1.00	45.03
42	CB	ALA	A	207	17.428	11.622	10.313	1.00	44.87
43	C	ALA	A	207	15.291	12.907	10.157	1.00	44.53
44	O	ALA	A	207	15.077	14.006	9.646	1.00	43.47
45	N	LYS	A	208	14.454	11.881	10.029	1.00	43.76
46	CA	LYS	A	208	13.226	12.011	9.251	1.00	42.20
47	CB	LYS	A	208	12.471	10.680	9.194	1.00	44.47
48	CG	LYS	A	208	11.537	10.576	7.990	1.00	45.43
49	CD	LYS	A	208	10.715	9.300	7.999	1.00	46.92
50	CE	LYS	A	208	9.660	9.328	9.093	1.00	48.09
51	NZ	LYS	A	208	8.799	8.114	9.059	1.00	49.24
52	C	LYS	A	208	12.330	13.086	9.852	1.00	41.19
53	O	LYS	A	208	11.658	13.818	9.128	1.00	40.18
54	N	ARG	A	209	12.328	13.174	11.179	1.00	38.94
55	CA	ARG	A	209	11.535	14.172	11.887	1.00	37.26
56	CB	ARG	A	209	11.745	14.022	13.398	1.00	39.88
57	CG	ARG	A	209	11.394	15.257	14.226	1.00	43.03
58	CD	ARG	A	209	9.901	15.543	14.240	1.00	45.71
59	NE	ARG	A	209	9.622	16.898	14.711	1.00	46.98

60	CZ	ARG	A	209	8.403	17.416	14.828	1.00	47.56
61	NH1	ARG	A	209	7.337	16.691	14.511	1.00	48.63
62	NH2	ARG	A	209	8.251	18.662	15.255	1.00	47.03
63	C	ARG	A	209	11.945	15.575	11.437	1.00	34.87
64	O	ARG	A	209	11.104	16.388	11.050	1.00	33.63
65	N	ILE	A	210	13.243	15.855	11.496	1.00	31.60
66	CA	ILE	A	210	13.759	17.156	11.086	1.00	28.45
67	CB	ILE	A	210	15.283	17.260	11.355	1.00	27.35
68	CG2	ILE	A	210	15.873	18.457	10.625	1.00	26.86
69	CG1	ILE	A	210	15.532	17.376	12.863	1.00	27.32
70	CD1	ILE	A	210	17.002	17.319	13.251	1.00	26.22
71	C	ILE	A	210	13.485	17.354	9.599	1.00	27.44
72	O	ILE	A	210	13.158	18.453	9.157	1.00	26.71
73	N	TYR	A	211	13.614	16.277	8.836	1.00	25.68
74	CA	TYR	A	211	13.370	16.335	7.403	1.00	26.73
75	CB	TYR	A	211	13.782	15.011	6.748	1.00	25.17
76	CG	TYR	A	211	13.657	14.971	5.236	1.00	27.92
77	CD1	TYR	A	211	13.862	16.116	4.464	1.00	27.10
78	CE1	TYR	A	211	13.787	16.071	3.073	1.00	27.40
79	CD2	TYR	A	211	13.372	13.775	4.573	1.00	28.20
80	CE2	TYR	A	211	13.296	13.721	3.180	1.00	29.60
81	CZ	TYR	A	211	13.506	14.875	2.437	1.00	28.67
82	OH	TYR	A	211	13.446	14.829	1.061	1.00	30.22
83	C	TYR	A	211	11.892	16.637	7.152	1.00	26.35
84	O	TYR	A	211	11.552	17.402	6.253	1.00	22.94
85	N	GLU	A	212	11.010	16.046	7.951	1.00	27.41
86	CA	GLU	A	212	9.586	16.299	7.778	1.00	27.15
87	CB	GLU	A	212	8.760	15.392	8.700	1.00	29.37
88	CG	GLU	A	212	8.870	13.917	8.324	1.00	32.72
89	CD	GLU	A	212	7.948	13.014	9.129	1.00	34.56
90	OE1	GLU	A	212	8.053	12.998	10.372	1.00	36.22
91	OE2	GLU	A	212	7.121	12.314	8.510	1.00	36.44
92	C	GLU	A	212	9.297	17.771	8.057	1.00	25.89

93	O	GLU	A	212	8.535	18.407	7.331	1.00	25.26
94	N	ALA	A	213	9.926	18.312	9.099	1.00	23.75
95	CA	ALA	A	213	9.746	19.712	9.461	1.00	22.66
96	CB	ALA	A	213	10.524	20.026	10.731	1.00	24.94
97	C	ALA	A	213	10.221	20.609	8.321	1.00	21.68
98	O	ALA	A	213	9.618	21.642	8.033	1.00	20.08
99	N	TYR	A	214	11.308	20.203	7.676	1.00	20.59
100	CA	TYR	A	214	11.873	20.956	6.563	1.00	20.21
101	CB	TYR	A	214	13.226	20.343	6.204	1.00	21.59
102	CG	TYR	A	214	13.895	20.850	4.950	1.00	20.23
103	CD1	TYR	A	214	13.565	20.322	3.701	1.00	21.49
104	CE1	TYR	A	214	14.259	20.692	2.557	1.00	20.65
105	CD2	TYR	A	214	14.933	21.779	5.019	1.00	19.83
106	CE2	TYR	A	214	15.635	22.156	3.877	1.00	20.40
107	CZ	TYR	A	214	15.295	21.603	2.651	1.00	20.09
108	OH	TYR	A	214	16.013	21.932	1.522	1.00	22.28
109	C	TYR	A	214	10.920	20.963	5.364	1.00	20.36
110	O	TYR	A	214	10.663	22.009	4.768	1.00	18.08
111	N	LEU	A	215	10.370	19.801	5.027	1.00	19.65
112	CA	LEU	A	215	9.453	19.720	3.896	1.00	21.64
113	CB	LEU	A	215	9.161	18.255	3.563	1.00	22.15
114	CG	LEU	A	215	10.347	17.450	3.031	1.00	23.81
115	CD1	LEU	A	215	9.934	15.993	2.840	1.00	24.83
116	CD2	LEU	A	215	10.824	18.055	1.711	1.00	24.52
117	C	LEU	A	215	8.144	20.462	4.161	1.00	21.59
118	O	LEU	A	215	7.521	20.994	3.246	1.00	22.21
119	N	LYS	A	216	7.730	20.509	5.419	1.00	21.23
120	CA	LYS	A	216	6.484	21.177	5.773	1.00	24.07
121	CB	LYS	A	216	5.974	20.611	7.107	1.00	27.04
122	CG	LYS	A	216	4.766	21.320	7.718	1.00	32.48
123	CD	LYS	A	216	5.177	22.541	8.536	1.00	34.35
124	CE	LYS	A	216	3.978	23.177	9.227	1.00	36.46
125	NZ	LYS	A	216	4.372	24.346	10.068	1.00	35.63

126	C	LYS	A	216	6.574	22.701	5.863	1.00	23.63
127	O	LYS	A	216	5.584	23.401	5.619	1.00	22.64
128	N	ASN	A	217	7.758	23.216	6.178	1.00	21.43
129	CA	ASN	A	217	7.922	24.655	6.371	1.00	21.60
130	CB	ASN	A	217	8.627	24.894	7.708	1.00	21.30
131	CG	ASN	A	217	7.734	24.576	8.887	1.00	21.85
132	OD1	ASN	A	217	6.763	25.286	9.144	1.00	21.90
133	ND2	ASN	A	217	8.041	23.493	9.596	1.00	21.00
134	C	ASN	A	217	8.576	25.515	5.304	1.00	20.24
135	O	ASN	A	217	8.485	26.741	5.369	1.00	21.01
136	N	PHE	A	218	9.226	24.902	4.324	1.00	19.71
137	CA	PHE	A	218	9.880	25.682	3.275	1.00	20.43
138	CB	PHE	A	218	11.352	25.283	3.158	1.00	19.13
139	CG	PHE	A	218	12.161	25.595	4.388	1.00	18.17
140	CD1	PHE	A	218	12.350	26.917	4.793	1.00	16.25
141	CD2	PHE	A	218	12.734	24.574	5.136	1.00	16.60
142	CE1	PHE	A	218	13.098	27.211	5.925	1.00	16.71
143	CE2	PHE	A	218	13.486	24.856	6.273	1.00	17.69
144	CZ	PHE	A	218	13.671	26.177	6.671	1.00	18.05
145	C	PHE	A	218	9.185	25.502	1.935	1.00	21.87
146	O	PHE	A	218	9.159	24.408	1.388	1.00	23.21
147	N	ASN	A	219	8.632	26.587	1.407	1.00	22.66
148	CA	ASN	A	219	7.927	26.530	0.136	1.00	23.56
149	CB	ASN	A	219	7.238	27.869	-0.135	1.00	26.95
150	CG	ASN	A	219	6.044	28.101	0.785	1.00	29.92
151	OD1	ASN	A	219	5.119	27.283	0.836	1.00	33.43
152	ND2	ASN	A	219	6.058	29.211	1.513	1.00	32.80
153	C	ASN	A	219	8.836	26.142	-1.026	1.00	23.59
154	O	ASN	A	219	8.374	25.604	-2.029	1.00	22.24
155	N	MET	A	220	10.129	26.413	-0.888	1.00	22.41
156	CA	MET	A	220	11.083	26.059	-1.927	1.00	23.18
157	CB	MET	A	220	11.713	27.316	-2.535	1.00	23.66
158	CG	MET	A	220	12.713	27.051	-3.664	1.00	25.31

159	SD	MET	A	220	11.971	26.305	-5.126	1.00	26.48
160	CE	MET	A	220	10.935	27.658	-5.694	1.00	24.83
161	C	MET	A	220	12.173	25.185	-1.329	1.00	23.23
162	O	MET	A	220	12.639	25.434	-0.214	1.00	23.23
163	N	ASN	A	221	12.549	24.147	-2.064	1.00	21.71
164	CA	ASN	A	221	13.610	23.245	-1.638	1.00	22.22
165	CB	ASN	A	221	13.049	22.029	-0.891	1.00	23.15
166	CG	ASN	A	221	12.074	21.224	-1.719	1.00	24.30
167	OD1	ASN	A	221	12.329	20.923	-2.880	1.00	25.96
168	ND2	ASN	A	221	10.954	20.851	-1.113	1.00	26.83
169	C	ASN	A	221	14.366	22.825	-2.889	1.00	22.09
170	O	ASN	A	221	13.994	23.218	-3.995	1.00	20.57
171	N	LYS	A	222	15.415	22.028	-2.724	1.00	20.59
172	CA	LYS	A	222	16.232	21.614	-3.858	1.00	20.89
173	CB	LYS	A	222	17.466	20.859	-3.361	1.00	21.48
174	CG	LYS	A	222	18.653	20.954	-4.297	1.00	20.77
175	CD	LYS	A	222	19.922	20.502	-3.602	1.00	21.19
176	CE	LYS	A	222	21.125	20.628	-4.507	1.00	21.09
177	NZ	LYS	A	222	22.361	20.180	-3.823	1.00	19.55
178	C	LYS	A	222	15.502	20.789	-4.914	1.00	20.69
179	O	LYS	A	222	15.678	21.022	-6.109	1.00	19.10
180	N	VAL	A	223	14.689	19.827	-4.493	1.00	20.29
181	CA	VAL	A	223	13.954	19.023	-5.463	1.00	23.64
182	CB	VAL	A	223	13.004	18.016	-4.776	1.00	25.30
183	CG1	VAL	A	223	12.236	17.229	-5.831	1.00	28.94
184	CG2	VAL	A	223	13.795	17.073	-3.900	1.00	28.35
185	C	VAL	A	223	13.125	19.930	-6.375	1.00	22.27
186	O	VAL	A	223	13.228	19.844	-7.600	1.00	22.87
187	N	LYS	A	224	12.314	20.797	-5.769	1.00	22.90
188	CA	LYS	A	224	11.460	21.724	-6.518	1.00	22.56
189	CB	LYS	A	224	10.640	22.604	-5.563	1.00	25.17
190	CG	LYS	A	224	9.512	21.908	-4.818	1.00	25.33
191	CD	LYS	A	224	8.688	22.947	-4.060	1.00	27.14

192	CE	LYS	A	224	7.467	22.352	-3.391	1.00	27.11
193	NZ	LYS	A	224	6.651	23.419	-2.738	1.00	25.12
194	C	LYS	A	224	12.254	22.635	-7.453	1.00	23.61
195	O	LYS	A	224	11.896	22.815	-8.622	1.00	22.28
196	N	ALA	A	225	13.329	23.215	-6.929	1.00	22.21
197	CA	ALA	A	225	14.174	24.112	-7.709	1.00	21.88
198	CB	ALA	A	225	15.237	24.738	-6.808	1.00	19.12
199	C	ALA	A	225	14.843	23.420	-8.896	1.00	22.78
200	O	ALA	A	225	14.863	23.960	-10.000	1.00	23.11
201	N	ARG	A	226	15.397	22.231	-8.675	1.00	23.76
202	CA	ARG	A	226	16.067	21.514	-9.753	1.00	26.20
203	CB	ARG	A	226	16.732	20.242	-9.215	1.00	27.83
204	CG	ARG	A	226	18.056	20.526	-8.517	1.00	28.58
205	CD	ARG	A	226	19.012	21.239	-9.467	1.00	32.23
206	NE	ARG	A	226	19.998	22.056	-8.766	1.00	34.36
207	CZ	ARG	A	226	19.683	23.053	-7.942	1.00	37.04
208	NH1	ARG	A	226	18.409	23.345	-7.713	1.00	39.09
209	NH2	ARG	A	226	20.636	23.772	-7.365	1.00	35.24
210	C	ARG	A	226	15.150	21.185	-10.926	1.00	27.67
211	O	ARG	A	226	15.590	21.176	-12.079	1.00	29.64
212	N	VAL	A	227	13.879	20.922	-10.639	1.00	27.53
213	CA	VAL	A	227	12.918	20.627	-11.697	1.00	28.83
214	CB	VAL	A	227	11.548	20.219	-11.120	1.00	30.09
215	CG1	VAL	A	227	10.500	20.186	-12.229	1.00	31.75
216	CG2	VAL	A	227	11.653	18.851	-10.464	1.00	31.01
217	C	VAL	A	227	12.728	21.878	-12.543	1.00	28.74
218	O	VAL	A	227	12.736	21.825	-13.775	1.00	27.81
219	N	ILE	A	228	12.561	23.010	-11.868	1.00	26.31
220	CA	ILE	A	228	12.365	24.283	-12.548	1.00	26.14
221	CB	ILE	A	228	12.050	25.398	-11.520	1.00	24.59
222	CG2	ILE	A	228	11.998	26.764	-12.200	1.00	23.06
223	CG1	ILE	A	228	10.720	25.094	-10.831	1.00	23.57
224	CD1	ILE	A	228	10.401	26.010	-9.661	1.00	25.78

225	C	ILE	A	228	13.592	24.671	-13.373	1.00	28.37
226	O	ILE	A	228	13.465	25.234	-14.462	1.00	27.38
227	N	LEU	A	229	14.776	24.355	-12.856	1.00	28.44
228	CA	LEU	A	229	16.027	24.684	-13.533	1.00	31.74
229	CB	LEU	A	229	17.156	24.801	-12.509	1.00	30.50
230	CG	LEU	A	229	17.045	25.984	-11.544	1.00	30.22
231	CD1	LEU	A	229	18.042	25.823	-10.405	1.00	29.46
232	CD2	LEU	A	229	17.290	27.279	-12.304	1.00	29.52
233	C	LEU	A	229	16.424	23.685	-14.616	1.00	34.68
234	O	LEU	A	229	17.281	23.974	-15.450	1.00	35.11
235	N	SER	A	230	15.808	22.509	-14.591	1.00	37.91
236	CA	SER	A	230	16.096	21.472	-15.574	1.00	42.67
237	CB	SER	A	230	17.416	20.768	-15.261	1.00	42.74
238	OG	SER	A	230	18.460	21.252	-16.085	1.00	44.54
239	C	SER	A	230	14.987	20.443	-15.629	1.00	45.44
240	O	SER	A	230	14.592	19.875	-14.613	1.00	46.52
241	N	GLY	A	231	14.491	20.203	-16.832	1.00	48.97
242	CA	GLY	A	231	13.427	19.242	-17.011	1.00	52.46
243	C	GLY	A	231	12.702	19.563	-18.294	1.00	55.01
244	O	GLY	A	231	12.343	18.658	-19.040	1.00	55.62
245	N	LYS	A	232	12.510	20.860	-18.542	1.00	57.05
246	CA	LYS	A	232	11.828	21.367	-19.732	1.00	58.42
247	CB	LYS	A	232	12.757	21.290	-20.945	1.00	59.37
248	CG	LYS	A	232	13.834	22.365	-20.980	1.00	58.74
249	CD	LYS	A	232	14.914	22.004	-21.989	1.00	59.57
250	CE	LYS	A	232	15.909	23.134	-22.205	1.00	59.20
251	NZ	LYS	A	232	15.454	24.073	-23.261	1.00	60.11
252	C	LYS	A	232	10.518	20.651	-20.036	1.00	59.28
253	O	LYS	A	232	9.537	21.285	-20.416	1.00	59.75
254	N	ALA	A	233	10.525	19.331	-19.869	1.00	60.20
255	CA	ALA	A	233	9.371	18.469	-20.097	1.00	60.65
256	CB	ALA	A	233	9.187	17.529	-18.907	1.00	60.60
257	C	ALA	A	233	8.110	19.284	-20.312	1.00	61.11

258	O	ALA	A	233	7.648	19.450	-21.442	1.00	61.12
259	N	SER	A	234	7.564	19.799	-19.217	1.00	61.07
260	CA	SER	A	234	6.360	20.609	-19.281	1.00	61.06
261	CB	SER	A	234	5.742	20.748	-17.885	1.00	61.00
262	OG	SER	A	234	4.582	21.563	-17.917	1.00	59.89
263	C	SER	A	234	6.687	21.988	-19.847	1.00	61.10
264	O	SER	A	234	7.344	22.107	-20.883	1.00	61.74
265	N	ASN	A	235	6.230	23.026	-19.157	1.00	60.20
266	CA	ASN	A	235	6.452	24.396	-19.590	1.00	59.10
267	CB	ASN	A	235	5.740	24.614	-20.934	1.00	58.65
268	CG	ASN	A	235	5.584	26.076	-21.296	1.00	58.90
269	OD1	ASN	A	235	4.628	26.728	-20.872	1.00	59.73
270	ND2	ASN	A	235	6.521	26.601	-22.081	1.00	58.39
271	C	ASN	A	235	5.952	25.349	-18.502	1.00	58.52
272	O	ASN	A	235	5.697	24.917	-17.377	1.00	59.67
273	N	ASN	A	236	5.807	26.629	-18.840	1.00	56.14
274	CA	ASN	A	236	5.393	27.666	-17.896	1.00	51.26
275	CB	ASN	A	236	4.356	27.117	-16.912	1.00	52.89
276	CG	ASN	A	236	4.033	28.087	-15.799	1.00	52.48
277	OD1	ASN	A	236	3.453	29.148	-16.028	1.00	52.78
278	ND2	ASN	A	236	4.413	27.729	-14.580	1.00	52.90
279	C	ASN	A	236	6.701	28.005	-17.179	1.00	47.02
280	O	ASN	A	236	6.751	28.137	-15.956	1.00	47.14
281	N	PRO	A	237	7.783	28.170	-17.966	1.00	42.04
282	CD	PRO	A	237	7.651	28.434	-19.410	1.00	41.47
283	CA	PRO	A	237	9.145	28.475	-17.529	1.00	38.16
284	CB	PRO	A	237	9.906	28.523	-18.846	1.00	38.68
285	CG	PRO	A	237	8.920	29.198	-19.729	1.00	39.97
286	C	PRO	A	237	9.338	29.755	-16.740	1.00	34.87
287	O	PRO	A	237	8.615	30.734	-16.921	1.00	34.21
288	N	PRO	A	238	10.338	29.760	-15.848	1.00	32.12
289	CD	PRO	A	238	11.273	28.667	-15.531	1.00	32.31
290	CA	PRO	A	238	10.617	30.943	-15.038	1.00	29.30

291	CB	PRO	A	238	11.741	30.470	-14.114	1.00	29.79
292	CG	PRO	A	238	12.436	29.411	-14.933	1.00	32.45
293	C	PRO	A	238	11.045	32.080	-15.960	1.00	27.36
294	O	PRO	A	238	11.745	31.861	-16.952	1.00	25.06
295	N	PHE	A	239	10.606	33.289	-15.637	1.00	24.30
296	CA	PHE	A	239	10.939	34.458	-16.431	1.00	23.14
297	CB	PHE	A	239	10.004	35.612	-16.083	1.00	25.05
298	CG	PHE	A	239	10.111	36.768	-17.022	1.00	26.31
299	CD1	PHE	A	239	9.483	36.729	-18.262	1.00	27.99
300	CD2	PHE	A	239	10.874	37.881	-16.691	1.00	27.41
301	CE1	PHE	A	239	9.615	37.784	-19.162	1.00	28.47
302	CE2	PHE	A	239	11.014	38.940	-17.583	1.00	28.03
303	CZ	PHE	A	239	10.382	38.891	-18.823	1.00	29.16
304	C	PHE	A	239	12.370	34.872	-16.133	1.00	22.55
305	O	PHE	A	239	12.723	35.087	-14.976	1.00	19.83
306	N	VAL	A	240	13.189	35.002	-17.171	1.00	22.23
307	CA	VAL	A	240	14.581	35.377	-16.974	1.00	21.89
308	CB	VAL	A	240	15.492	34.735	-18.051	1.00	23.08
309	CG1	VAL	A	240	16.919	35.265	-17.916	1.00	22.71
310	CG2	VAL	A	240	15.487	33.217	-17.889	1.00	22.78
311	C	VAL	A	240	14.813	36.884	-16.959	1.00	22.84
312	O	VAL	A	240	14.387	37.613	-17.861	1.00	22.43
313	N	ILE	A	241	15.482	37.340	-15.905	1.00	20.77
314	CA	ILE	A	241	15.817	38.745	-15.740	1.00	20.91
315	CB	ILE	A	241	15.496	39.223	-14.306	1.00	20.98
316	CG2	ILE	A	241	15.897	40.687	-14.137	1.00	19.06
317	CG1	ILE	A	241	13.999	39.039	-14.028	1.00	19.24
318	CD1	ILE	A	241	13.607	39.288	-12.574	1.00	21.68
319	C	ILE	A	241	17.317	38.844	-16.006	1.00	21.63
320	O	ILE	A	241	18.137	38.438	-15.172	1.00	19.53
321	N	HIS	A	242	17.673	39.362	-17.181	1.00	20.99
322	CA	HIS	A	242	19.077	39.476	-17.568	1.00	22.26
323	CB	HIS	A	242	19.355	38.567	-18.769	1.00	24.28

324	CG	HIS	A	242	18.588	38.937	-19.998	1.00	24.97
325	CD2	HIS	A	242	17.459	38.415	-20.534	1.00	25.77
326	ND1	HIS	A	242	18.951	39.986	-20.816	1.00	27.65
327	CE1	HIS	A	242	18.077	40.096	-21.800	1.00	25.99
328	NE2	HIS	A	242	17.162	39.156	-21.653	1.00	26.18
329	C	HIS	A	242	19.537	40.902	-17.868	1.00	23.10
330	O	HIS	A	242	20.721	41.135	-18.111	1.00	21.51
331	N	ASP	A	243	18.600	41.847	-17.848	1.00	23.64
332	CA	ASP	A	243	18.910	43.255	-18.074	1.00	26.61
333	CB	ASP	A	243	19.170	43.546	-19.561	1.00	27.87
334	CG	ASP	A	243	17.972	43.258	-20.445	1.00	29.61
335	OD1	ASP	A	243	16.851	43.097	-19.921	1.00	28.47
336	OD2	ASP	A	243	18.157	43.206	-21.683	1.00	31.76
337	C	ASP	A	243	17.792	44.150	-17.553	1.00	27.23
338	O	ASP	A	243	16.800	43.668	-17.006	1.00	25.64
339	N	MET	A	244	17.953	45.457	-17.727	1.00	28.20
340	CA	MET	A	244	16.964	46.414	-17.243	1.00	28.88
341	CB	MET	A	244	17.466	47.838	-17.483	1.00	31.16
342	CG	MET	A	244	18.749	48.140	-16.733	1.00	33.46
343	SD	MET	A	244	18.511	48.081	-14.932	1.00	36.77
344	CE	MET	A	244	19.258	49.667	-14.476	1.00	37.18
345	C	MET	A	244	15.571	46.241	-17.837	1.00	28.34
346	O	MET	A	244	14.567	46.411	-17.138	1.00	27.10
347	N	GLU	A	245	15.500	45.895	-19.118	1.00	28.20
348	CA	GLU	A	245	14.206	45.709	-19.760	1.00	27.38
349	CB	GLU	A	245	14.375	45.546	-21.274	1.00	30.74
350	CG	GLU	A	245	13.072	45.246	-21.999	1.00	34.46
351	CD	GLU	A	245	13.226	45.229	-23.510	1.00	37.18
352	OE1	GLU	A	245	14.109	44.505	-24.016	1.00	38.99
353	OE2	GLU	A	245	12.455	45.936	-24.191	1.00	39.82
354	C	GLU	A	245	13.452	44.508	-19.189	1.00	26.77
355	O	GLU	A	245	12.274	44.615	-18.844	1.00	24.55
356	N	THR	A	246	14.126	43.366	-19.086	1.00	25.14

357	CA	THR	A	246	13.485	42.169	-18.550	1.00	22.92
358	CB	THR	A	246	14.342	40.909	-18.802	1.00	22.22
359	OG1	THR	A	246	15.686	41.135	-18.362	1.00	20.92
360	CG2	THR	A	246	14.352	40.571	-20.288	1.00	22.08
361	C	THR	A	246	13.172	42.299	-17.058	1.00	22.64
362	O	THR	A	246	12.284	41.615	-16.545	1.00	21.75
363	N	LEU	A	247	13.896	43.171	-16.360	1.00	21.77
364	CA	LEU	A	247	13.630	43.386	-14.936	1.00	20.25
365	CB	LEU	A	247	14.698	44.278	-14.289	1.00	20.20
366	CG	LEU	A	247	14.339	44.724	-12.861	1.00	18.26
367	CD1	LEU	A	247	14.285	43.498	-11.941	1.00	19.55
368	CD2	LEU	A	247	15.367	45.723	-12.342	1.00	17.68
369	C	LEU	A	247	12.280	44.081	-14.833	1.00	20.44
370	O	LEU	A	247	11.417	43.678	-14.064	1.00	19.24
371	N	CYS	A	248	12.094	45.126	-15.630	1.00	20.05
372	CA	CYS	A	248	10.833	45.856	-15.606	1.00	22.13
373	CB	CYS	A	248	10.904	47.076	-16.536	1.00	22.88
374	SG	CYS	A	248	12.090	48.355	-16.013	1.00	28.89
375	C	CYS	A	248	9.681	44.939	-16.016	1.00	22.46
376	O	CYS	A	248	8.594	45.020	-15.452	1.00	23.21
377	N	MET	A	249	9.921	44.067	-16.994	1.00	24.21
378	CA	MET	A	249	8.889	43.139	-17.465	1.00	25.70
379	CB	MET	A	249	9.392	42.333	-18.668	1.00	28.67
380	CG	MET	A	249	9.874	43.175	-19.847	1.00	34.04
381	SD	MET	A	249	10.480	42.192	-21.255	1.00	38.98
382	CE	MET	A	249	10.112	43.318	-22.621	1.00	38.27
383	C	MET	A	249	8.504	42.178	-16.342	1.00	25.87
384	O	MET	A	249	7.323	41.924	-16.098	1.00	25.43
385	N	ALA	A	250	9.511	41.646	-15.657	1.00	24.88
386	CA	ALA	A	250	9.268	40.720	-14.559	1.00	23.76
387	CB	ALA	A	250	10.590	40.188	-14.022	1.00	22.98
388	C	ALA	A	250	8.482	41.406	-13.446	1.00	22.99
389	O	ALA	A	250	7.546	40.829	-12.889	1.00	23.42

390	N	GLU	A	251	8.863	42.639	-13.121	1.00	22.90
391	CA	GLU	A	251	8.176	43.387	-12.075	1.00	23.30
392	CB	GLU	A	251	8.840	44.756	-11.865	1.00	23.04
393	CG	GLU	A	251	10.269	44.676	-11.336	1.00	23.77
394	CD	GLU	A	251	10.969	46.025	-11.283	1.00	25.32
395	OE1	GLU	A	251	10.914	46.766	-12.288	1.00	26.09
396	OE2	GLU	A	251	11.590	46.341	-10.247	1.00	24.65
397	C	GLU	A	251	6.713	43.572	-12.465	1.00	24.60
398	O	GLU	A	251	5.815	43.401	-11.646	1.00	23.99
399	N	LYS	A	252	6.482	43.911	-13.728	1.00	26.88
400	CA	LYS	A	252	5.129	44.120	-14.227	1.00	29.38
401	CB	LYS	A	252	5.163	44.406	-15.729	1.00	31.11
402	CG	LYS	A	252	3.792	44.688	-16.321	1.00	34.55
403	CD	LYS	A	252	3.707	46.086	-16.917	1.00	38.59
404	CE	LYS	A	252	4.142	47.146	-15.921	1.00	40.59
405	NZ	LYS	A	252	5.625	47.202	-15.814	1.00	42.89
406	C	LYS	A	252	4.229	42.912	-13.965	1.00	30.43
407	O	LYS	A	252	3.045	43.059	-13.656	1.00	30.61
408	N	THR	A	253	4.797	41.717	-14.083	1.00	31.64
409	CA	THR	A	253	4.035	40.492	-13.879	1.00	32.66
410	CB	THR	A	253	4.508	39.385	-14.840	1.00	34.32
411	OG1	THR	A	253	4.522	39.884	-16.185	1.00	37.49
412	CG2	THR	A	253	3.564	38.191	-14.767	1.00	34.76
413	C	THR	A	253	4.076	39.923	-12.459	1.00	32.57
414	O	THR	A	253	3.033	39.621	-11.876	1.00	33.27
415	N	LEU	A	254	5.275	39.784	-11.904	1.00	31.54
416	CA	LEU	A	254	5.441	39.208	-10.572	1.00	31.84
417	CB	LEU	A	254	6.805	38.522	-10.489	1.00	32.07
418	CG	LEU	A	254	6.933	37.131	-11.126	1.00	33.07
419	CD1	LEU	A	254	5.781	36.849	-12.083	1.00	32.88
420	CD2	LEU	A	254	8.271	37.040	-11.833	1.00	32.53
421	C	LEU	A	254	5.256	40.128	-9.367	1.00	32.52
422	O	LEU	A	254	4.770	39.690	-8.321	1.00	31.50

423	N	VAL	A	255	5.654	41.389	-9.501	1.00	32.08
424	CA	VAL	A	255	5.514	42.353	-8.413	1.00	32.49
425	CB	VAL	A	255	6.870	42.614	-7.710	1.00	32.30
426	CG1	VAL	A	255	6.698	43.659	-6.620	1.00	33.97
427	CG2	VAL	A	255	7.393	41.322	-7.095	1.00	33.63
428	C	VAL	A	255	4.988	43.650	-9.017	1.00	33.56
429	O	VAL	A	255	5.664	44.680	-9.018	1.00	32.17
430	N	ALA	A	256	3.766	43.571	-9.532	1.00	34.97
431	CA	ALA	A	256	3.092	44.685	-10.192	1.00	35.76
432	CB	ALA	A	256	1.636	44.310	-10.438	1.00	37.47
433	C	ALA	A	256	3.162	46.065	-9.529	1.00	37.14
434	O	ALA	A	256	3.127	47.083	-10.224	1.00	35.98
435	N	LYS	A	257	3.267	46.114	-8.203	1.00	37.87
436	CA	LYS	A	257	3.310	47.404	-7.509	1.00	39.85
437	CB	LYS	A	257	3.154	47.210	-5.995	1.00	39.30
438	CG	LYS	A	257	3.135	48.531	-5.218	1.00	40.41
439	CD	LYS	A	257	3.092	48.326	-3.708	1.00	41.21
440	CE	LYS	A	257	1.717	47.890	-3.228	1.00	42.93
441	NZ	LYS	A	257	0.674	48.923	-3.504	1.00	44.25
442	C	LYS	A	257	4.553	48.260	-7.772	1.00	40.87
443	O	LYS	A	257	4.477	49.489	-7.764	1.00	41.16
444	N	LEU	A	258	5.693	47.618	-7.999	1.00	41.92
445	CA	LEU	A	258	6.934	48.347	-8.241	1.00	43.90
446	CB	LEU	A	258	8.133	47.431	-8.002	1.00	43.36
447	CG	LEU	A	258	8.106	46.627	-6.702	1.00	42.94
448	CD1	LEU	A	258	9.465	45.980	-6.481	1.00	42.92
449	CD2	LEU	A	258	7.756	47.541	-5.536	1.00	43.54
450	C	LEU	A	258	7.021	48.917	-9.647	1.00	45.44
451	O	LEU	A	258	8.118	49.189	-10.142	1.00	45.30
452	N	VAL	A	259	5.874	49.138	-10.277	1.00	47.08
453	CA	VAL	A	259	5.899	49.643	-11.634	1.00	49.10
454	CB	VAL	A	259	5.984	48.463	-12.612	1.00	49.12
455	CG1	VAL	A	259	4.606	47.839	-12.800	1.00	49.41

456	CG2	VAL	A	259	6.587	48.926	-13.921	1.00	49.20
457	C	VAL	A	259	4.716	50.538	-12.012	1.00	50.30
458	O	VAL	A	259	4.459	50.771	-13.194	1.00	50.13
459	N	ALA	A	260	4.010	51.065	-11.016	1.00	51.85
460	CA	ALA	A	260	2.860	51.925	-11.304	1.00	53.91
461	CB	ALA	A	260	1.627	51.065	-11.582	1.00	53.84
462	C	ALA	A	260	2.542	52.938	-10.207	1.00	55.04
463	O	ALA	A	260	1.443	53.496	-10.173	1.00	55.68
464	N	ASN	A	261	3.496	53.182	-9.314	1.00	55.70
465	CA	ASN	A	261	3.277	54.134	-8.225	1.00	57.57
466	CB	ASN	A	261	3.064	53.389	-6.905	1.00	20.38
467	CG	ASN	A	261	1.795	52.578	-6.902	1.00	20.38
468	OD1	ASN	A	261	1.812	51.370	-7.162	1.00	20.38
469	ND2	ASN	A	261	0.670	53.245	-6.633	1.00	20.38
470	C	ASN	A	261	4.414	55.132	-8.048	1.00	58.36
471	O	ASN	A	261	4.672	55.595	-6.937	1.00	58.74
472	N	GLY	A	262	5.081	55.473	-9.145	1.00	20.38
473	CA	GLY	A	262	6.204	56.394	-9.063	1.00	20.38
474	C	GLY	A	262	7.442	55.570	-8.751	1.00	20.38
475	O	GLY	A	262	8.576	56.039	-8.883	1.00	20.38
476	N	ILE	A	263	7.213	54.319	-8.352	1.00	58.34
477	CA	ILE	A	263	8.300	53.404	-8.015	1.00	57.76
478	CB	ILE	A	263	7.787	52.149	-7.293	1.00	58.40
479	CG2	ILE	A	263	8.946	51.405	-6.661	1.00	58.51
480	CG1	ILE	A	263	6.764	52.524	-6.225	1.00	58.87
481	CD1	ILE	A	263	6.170	51.325	-5.498	1.00	59.43
482	C	ILE	A	263	9.054	52.942	-9.254	1.00	57.27
483	O	ILE	A	263	10.193	52.497	-9.157	1.00	57.93
484	N	GLN	A	264	8.410	53.027	-10.415	1.00	55.75
485	CA	GLN	A	264	9.038	52.596	-11.658	1.00	54.43
486	CB	GLN	A	264	8.116	52.845	-12.849	1.00	54.62
487	CG	GLN	A	264	7.654	54.270	-13.006	1.00	54.62
488	CD	GLN	A	264	6.221	54.465	-12.572	1.00	54.37

489	OE1	GLN	A	264	5.896	54.391	-11.390	1.00	54.65
490	NE2	GLN	A	264	5.347	54.710	-13.539	1.00	53.99
491	C	GLN	A	264	10.378	53.265	-11.896	1.00	53.23
492	O	GLN	A	264	11.164	52.791	-12.714	1.00	53.33
493	N	ASN	A	265	10.648	54.369	-11.203	1.00	51.79
494	CA	ASN	A	265	11.943	54.991	-11.390	1.00	50.16
495	CB	ASN	A	265	11.889	56.162	-12.357	1.00	52.29
496	CG	ASN	A	265	13.036	56.120	-13.366	1.00	54.63
497	OD1	ASN	A	265	13.488	57.150	-13.866	1.00	56.51
498	ND2	ASN	A	265	13.504	54.914	-13.673	1.00	55.84
499	C	ASN	A	265	12.728	55.397	-10.164	1.00	47.37
500	O	ASN	A	265	13.251	56.509	-10.078	1.00	47.22
501	N	LYS	A	266	12.765	54.494	-9.195	1.00	43.69
502	CA	LYS	A	266	13.617	54.669	-8.039	1.00	38.70
503	CB	LYS	A	266	13.077	53.921	-6.817	1.00	39.95
504	CG	LYS	A	266	11.973	54.657	-6.077	1.00	41.04
505	CD	LYS	A	266	11.700	54.020	-4.721	1.00	42.78
506	CE	LYS	A	266	10.676	54.817	-3.920	1.00	43.67
507	NZ	LYS	A	266	10.422	54.216	-2.578	1.00	44.37
508	C	LYS	A	266	14.628	53.824	-8.797	1.00	35.85
509	O	LYS	A	266	14.207	52.956	-9.570	1.00	32.72
510	N	GLU	A	267	15.926	54.045	-8.653	1.00	33.11
511	CA	GLU	A	267	16.809	53.225	-9.468	1.00	30.98
512	CB	GLU	A	267	18.281	53.630	-9.312	1.00	34.18
513	CG	GLU	A	267	18.846	53.674	-7.923	1.00	36.39
514	CD	GLU	A	267	20.153	54.445	-7.890	1.00	36.02
515	OE1	GLU	A	267	21.030	54.183	-8.740	1.00	36.54
516	OE2	GLU	A	267	20.305	55.317	-7.014	1.00	38.61
517	C	GLU	A	267	16.604	51.732	-9.252	1.00	29.49
518	O	GLU	A	267	16.183	51.288	-8.184	1.00	26.80
519	N	ALA	A	268	16.868	50.970	-10.306	1.00	26.80
520	CA	ALA	A	268	16.702	49.526	-10.293	1.00	27.28
521	CB	ALA	A	268	17.312	48.937	-11.549	1.00	26.70

522	C	ALA	A	268	17.280	48.838	-9.064	1.00	24.93
523	O	ALA	A	268	16.620	47.991	-8.459	1.00	23.64
524	N	GLU	A	269	18.504	49.199	-8.685	1.00	22.59
525	CA	GLU	A	269	19.126	48.561	-7.536	1.00	22.23
526	CB	GLU	A	269	20.539	49.116	-7.274	1.00	23.67
527	CG	GLU	A	269	20.876	50.450	-7.915	1.00	27.55
528	CD	GLU	A	269	21.024	50.367	-9.423	1.00	24.59
529	OE1	GLU	A	269	20.048	50.679	-10.116	1.00	26.10
530	OE2	GLU	A	269	22.109	49.985	-9.918	1.00	26.97
531	C	GLU	A	269	18.291	48.654	-6.263	1.00	22.57
532	O	GLU	A	269	18.307	47.737	-5.447	1.00	21.72
533	N	VAL	A	270	17.553	49.746	-6.095	1.00	21.59
534	CA	VAL	A	270	16.728	49.911	-4.899	1.00	21.26
535	CB	VAL	A	270	16.290	51.377	-4.730	1.00	23.06
536	CG1	VAL	A	270	15.279	51.504	-3.604	1.00	25.08
537	CG2	VAL	A	270	17.509	52.238	-4.430	1.00	25.52
538	C	VAL	A	270	15.502	49.001	-4.950	1.00	19.49
539	O	VAL	A	270	15.064	48.468	-3.921	1.00	18.78
540	N	ARG	A	271	14.956	48.820	-6.149	1.00	18.65
541	CA	ARG	A	271	13.799	47.948	-6.340	1.00	17.90
542	CB	ARG	A	271	13.238	48.104	-7.760	1.00	18.81
543	CG	ARG	A	271	12.207	49.209	-7.891	1.00	23.01
544	CD	ARG	A	271	12.325	49.944	-9.206	1.00	23.63
545	NE	ARG	A	271	12.388	49.055	-10.366	1.00	21.82
546	CZ	ARG	A	271	12.893	49.422	-11.539	1.00	23.69
547	NH1	ARG	A	271	13.374	50.649	-11.693	1.00	25.06
548	NH2	ARG	A	271	12.923	48.573	-12.554	1.00	24.09
549	C	ARG	A	271	14.219	46.498	-6.102	1.00	17.66
550	O	ARG	A	271	13.528	45.743	-5.420	1.00	16.97
551	N	ILE	A	272	15.361	46.118	-6.662	1.00	17.24
552	CA	ILE	A	272	15.879	44.762	-6.499	1.00	16.58
553	CB	ILE	A	272	17.151	44.558	-7.346	1.00	17.41
554	CG2	ILE	A	272	17.842	43.238	-6.962	1.00	17.49

555	CG1	ILE	A	272	16.772	44.568	-8.832	1.00	17.66
556	CD1	ILE	A	272	17.954	44.508	-9.785	1.00	19.17
557	C	ILE	A	272	16.193	44.505	-5.026	1.00	16.90
558	O	ILE	A	272	15.893	43.434	-4.499	1.00	16.85
559	N	PHE	A	273	16.779	45.497	-4.361	1.00	14.57
560	CA	PHE	A	273	17.114	45.364	-2.943	1.00	13.82
561	CB	PHE	A	273	17.884	46.591	-2.456	1.00	14.33
562	CG	PHE	A	273	18.485	46.427	-1.086	1.00	16.86
563	CD1	PHE	A	273	19.604	45.626	-0.899	1.00	17.16
564	CD2	PHE	A	273	17.937	47.078	0.012	1.00	16.21
565	CE1	PHE	A	273	20.174	45.475	0.356	1.00	18.94
566	CE2	PHE	A	273	18.498	46.936	-1.275	1.00	19.15
567	CZ	PHE	A	273	19.621	46.133	1.448	1.00	20.18
568	C	PHE	A	273	15.850	45.203	-2.102	1.00	14.30
569	O	PHE	A	273	15.860	44.505	-1.096	1.00	15.47
570	N	HIS	A	274	14.768	45.874	-2.496	1.00	14.52
571	CA	HIS	A	274	13.519	45.756	-1.758	1.00	15.32
572	CB	HIS	A	274	12.455	46.695	-2.330	1.00	16.74
573	CG	HIS	A	274	11.139	46.603	-1.624	1.00	18.93
574	CD2	HIS	A	274	9.960	46.057	-2.003	1.00	21.47
575	ND1	HIS	A	274	10.954	47.061	-0.337	1.00	19.40
576	CE1	HIS	A	274	9.718	46.799	0.047	1.00	21.96
577	NE2	HIS	A	274	9.093	46.189	-0.945	1.00	23.33
578	C	HIS	A	274	13.033	44.312	-1.878	1.00	14.53
579	O	HIS	A	274	12.605	43.706	-0.903	1.00	15.83
580	N	CYS	A	275	13.096	43.769	-3.088	1.00	14.60
581	CA	CYS	A	275	12.674	42.388	-3.323	1.00	14.94
582	CB	CYS	A	275	12.721	42.064	-4.816	1.00	14.09
583	SG	CYS	A	275	11.470	42.950	-5.767	1.00	16.01
584	C	CYS	A	275	13.558	41.414	-2.544	1.00	14.97
585	O	CYS	A	275	13.090	40.366	-2.099	1.00	13.78
586	N	CYS	A	276	14.836	41.748	-2.383	1.00	15.23
587	CA	CYS	A	276	15.740	40.880	-1.625	1.00	13.47

588	CB	CYS	A	276	17.180	41.409	-1.667	1.00	15.89
589	SG	CYS	A	276	17.996	41.235	-3.256	1.00	15.55
590	C	CYS	A	276	15.265	40.844	-0.176	1.00	15.09
591	O	CYS	A	276	15.264	39.789	0.467	1.00	15.43
592	N	GLN	A	277	14.861	42.005	0.332	1.00	13.05
593	CA	GLN	A	277	14.379	42.105	1.707	1.00	14.74
594	CB	GLN	A	277	14.150	43.564	2.100	1.00	16.57
595	CG	GLN	A	277	15.418	44.386	2.205	1.00	18.11
596	CD	GLN	A	277	15.231	45.597	3.093	1.00	20.26
597	OE1	GLN	A	277	14.949	45.465	4.286	1.00	22.83
598	NE2	GLN	A	277	15.383	46.784	2.520	1.00	22.10
599	C	GLN	A	277	13.086	41.339	1.909	1.00	14.38
600	O	GLN	A	277	12.905	40.665	2.924	1.00	14.08
601	N	CYS	A	278	12.175	41.451	0.949	1.00	14.67
602	CA	CYS	A	278	10.911	40.741	1.062	1.00	15.04
603	CB	CYS	A	278	9.994	41.091	-0.110	1.00	16.30
604	SG	CYS	A	278	9.396	42.797	-0.061	1.00	22.25
605	C	CYS	A	278	11.192	39.245	1.093	1.00	14.70
606	O	CYS	A	278	10.593	38.505	1.868	1.00	14.34
607	N	THR	A	279	12.119	38.813	0.244	1.00	14.73
608	CA	THR	A	279	12.517	37.412	0.164	1.00	14.32
609	CB	THR	A	279	13.514	37.211	-0.997	1.00	15.37
610	OG1	THR	A	279	12.888	37.603	-2.230	1.00	13.87
611	CG2	THR	A	279	13.943	35.748	-1.094	1.00	14.11
612	C	THR	A	279	13.135	36.946	1.488	1.00	14.08
613	O	THR	A	279	12.771	35.897	2.029	1.00	13.41
614	N	SER	A	280	14.057	37.732	2.028	1.00	12.61
615	CA	SER	A	280	14.672	37.371	3.303	1.00	12.61
616	CB	SER	A	280	15.775	38.361	3.657	1.00	12.19
617	OG	SER	A	280	16.915	38.120	2.860	1.00	11.40
618	C	SER	A	280	13.660	37.309	4.450	1.00	12.67
619	O	SER	A	280	13.726	36.413	5.283	1.00	12.90
620	N	VAL	A	281	12.720	38.249	4.492	1.00	13.57

621	CA	VAL	A	281	11.723	38.249	5.563	1.00	13.84
622	CB	VAL	A	281	10.790	39.480	5.461	1.00	15.55
623	CG1	VAL	A	281	9.555	39.303	6.345	1.00	17.55
624	CG2	VAL	A	281	11.558	40.721	5.895	1.00	16.53
625	C	VAL	A	281	10.911	36.961	5.533	1.00	15.35
626	O	VAL	A	281	10.639	36.366	6.575	1.00	14.98
627	N	GLU	A	282	10.546	36.522	4.334	1.00	16.73
628	CA	GLU	A	282	9.777	35.292	4.182	1.00	16.47
629	CB	GLU	A	282	9.338	35.113	2.726	1.00	19.03
630	CG	GLU	A	282	8.344	36.159	2.235	1.00	22.45
631	CD	GLU	A	282	6.924	35.908	2.727	1.00	27.72
632	OE1	GLU	A	282	6.724	34.990	3.558	1.00	28.03
633	OE2	GLU	A	282	6.009	36.635	2.279	1.00	27.23
634	C	GLU	A	282	10.603	34.088	4.612	1.00	15.29
635	O	GLU	A	282	10.099	33.192	5.282	1.00	14.93
636	N	THR	A	283	11.877	34.066	4.235	1.00	13.72
637	CA	THR	A	283	12.727	32.937	4.590	1.00	13.42
638	CB	THR	A	283	14.070	33.003	3.843	1.00	13.57
639	OG1	THR	A	283	13.822	33.115	2.433	1.00	13.65
640	CG2	THR	A	283	14.878	31.738	4.091	1.00	13.97
641	C	THR	A	283	12.961	32.876	6.097	1.00	13.92
642	O	THR	A	283	12.956	31.796	6.687	1.00	15.10
643	N	VAL	A	284	13.159	34.034	6.723	1.00	14.12
644	CA	VAL	A	284	13.359	34.074	8.176	1.00	14.58
645	CB	VAL	A	284	13.612	35.508	8.674	1.00	14.45
646	CG1	VAL	A	284	13.507	35.559	10.200	1.00	15.36
647	CG2	VAL	A	284	14.976	35.980	8.225	1.00	15.78
648	C	VAL	A	284	12.097	33.541	8.861	1.00	14.26
649	O	VAL	A	284	12.165	32.827	9.870	1.00	14.04
650	N	THR	A	285	10.944	33.900	8.309	1.00	15.03
651	CA	THR	A	285	9.670	33.458	8.866	1.00	16.55
652	CB	THR	A	285	8.493	34.139	8.133	1.00	17.70
653	OG1	THR	A	285	8.641	35.566	8.224	1.00	18.26

654	CG2	THR	A	285	7.160	33.743	8.759	1.00	18.59
655	C	THR	A	285	9.551	31.931	8.775	1.00	16.67
656	O	THR	A	285	9.108	31.279	9.719	1.00	15.85
657	N	GLU	A	286	9.959	31.354	7.648	1.00	16.45
658	CA	GLU	A	286	9.897	29.897	7.489	1.00	14.59
659	CB	GLU	A	286	10.199	29.492	6.040	1.00	17.05
660	CG	GLU	A	286	9.201	29.983	5.025	1.00	19.53
661	CD	GLU	A	286	9.539	29.509	3.621	1.00	21.27
662	OE1	GLU	A	286	10.740	29.424	3.291	1.00	24.29
663	OE2	GLU	A	286	8.606	29.235	2.846	1.00	26.60
664	C	GLU	A	286	10.894	29.184	8.410	1.00	15.53
665	O	GLU	A	286	10.598	28.121	8.964	1.00	14.95
666	N	LEU	A	287	12.080	29.767	8.559	1.00	14.15
667	CA	LEU	A	287	13.117	29.183	9.404	1.00	14.54
668	CB	LEU	A	287	14.418	29.977	9.244	1.00	13.35
669	CG	LEU	A	287	15.286	29.532	8.062	1.00	13.79
670	CD1	LEU	A	287	16.277	30.630	7.670	1.00	14.77
671	CD2	LEU	A	287	16.029	28.253	8.452	1.00	15.41
672	C	LEU	A	287	12.684	29.185	10.863	1.00	15.65
673	O	LEU	A	287	13.017	28.277	11.627	1.00	15.76
674	N	THR	A	288	11.946	30.219	11.245	1.00	16.74
675	CA	THR	A	288	11.468	30.342	12.616	1.00	17.31
676	CB	THR	A	288	10.814	31.724	12.830	1.00	17.24
677	OG1	THR	A	288	11.821	32.736	12.693	1.00	18.00
678	CG2	THR	A	288	10.180	31.832	14.221	1.00	18.26
679	C	THR	A	288	10.484	29.211	12.913	1.00	18.94
680	O	THR	A	288	10.520	28.615	13.995	1.00	18.36
681	N	GLU	A	289	9.617	28.906	11.947	1.00	18.64
682	CA	GLU	A	289	8.654	27.824	12.120	1.00	19.64
683	CB	GLU	A	289	7.591	27.868	11.019	1.00	20.78
684	CG	GLU	A	289	6.701	29.088	11.102	1.00	24.51
685	CD	GLU	A	289	5.978	29.170	12.429	1.00	27.16
686	OE1	GLU	A	289	5.151	28.276	12.705	1.00	28.65

687	OE2	GLU	A	289	6.245	30.118	13.197	1.00	29.29
688	C	GLU	A	289	9.378	26.482	12.094	1.00	19.12
689	O	GLU	A	289	8.998	25.550	12.802	1.00	19.43
690	N	PHE	A	290	10.414	26.381	11.263	1.00	18.63
691	CA	PHE	A	290	11.215	25.158	11.177	1.00	18.56
692	CB	PHE	A	290	12.295	25.304	10.097	1.00	18.22
693	CG	PHE	A	290	13.295	24.178	10.074	1.00	16.52
694	CD1	PHE	A	290	12.913	22.894	9.702	1.00	15.73
695	CD2	PHE	A	290	14.628	24.411	10.407	1.00	16.62
696	CE1	PHE	A	290	13.844	21.854	9.657	1.00	16.62
697	CE2	PHE	A	290	15.564	23.387	10.367	1.00	16.63
698	CZ	PHE	A	290	15.170	22.097	9.987	1.00	16.10
699	C	PHE	A	290	11.894	24.898	12.525	1.00	19.02
700	O	PHE	A	290	11.856	23.783	13.049	1.00	19.20
701	N	ALA	A	291	12.529	25.931	13.073	1.00	19.85
702	CA	ALA	A	291	13.226	25.800	14.353	1.00	19.89
703	CB	ALA	A	291	13.856	27.130	14.746	1.00	20.05
704	C	ALA	A	291	12.270	25.337	15.449	1.00	21.19
705	O	ALA	A	291	12.623	24.499	16.283	1.00	19.62
706	N	LYS	A	292	11.064	25.897	15.447	1.00	21.75
707	CA	LYS	A	292	10.053	25.545	16.439	1.00	23.62
708	CB	LYS	A	292	8.802	26.407	16.245	1.00	22.82
709	CG	LYS	A	292	8.959	27.846	16.715	1.00	27.26
710	CD	LYS	A	292	7.821	28.738	16.214	1.00	30.13
711	CE	LYS	A	292	6.452	28.165	16.544	1.00	32.35
712	NZ	LYS	A	292	6.234	28.014	18.007	1.00	36.87
713	C	LYS	A	292	9.686	24.070	16.346	1.00	24.64
714	O	LYS	A	292	9.150	23.493	17.295	1.00	24.87
715	N	ALA	A	293	9.983	23.460	15.202	1.00	24.73
716	CA	ALA	A	293	9.684	22.051	14.985	1.00	24.93
717	CB	ALA	A	293	9.190	21.840	13.562	1.00	24.81
718	C	ALA	A	293	10.871	21.129	15.274	1.00	24.71
719	O	ALA	A	293	10.750	19.909	15.185	1.00	23.86

720	N	ILE	A	294	12.024	21.704	15.606	1.00	23.98
721	CA	ILE	A	294	13.188	20.885	15.925	1.00	22.06
722	CB	ILE	A	294	14.511	21.661	15.764	1.00	21.52
723	CG2	ILE	A	294	15.684	20.769	16.166	1.00	20.29
724	CG1	ILE	A	294	14.687	22.112	14.310	1.00	18.78
725	CD1	ILE	A	294	15.938	22.940	14.085	1.00	20.43
726	C	ILE	A	294	13.065	20.448	17.383	1.00	23.55
727	O	ILE	A	294	13.023	21.284	18.284	1.00	22.86
728	N	PRO	A	295	13.006	19.130	17.629	1.00	24.07
729	CD	PRO	A	295	13.131	18.036	16.648	1.00	23.94
730	CA	PRO	A	295	12.885	18.592	18.989	1.00	24.71
731	CB	PRO	A	295	13.284	17.135	18.808	1.00	24.70
732	CG	PRO	A	295	12.728	16.824	17.458	1.00	25.44
733	C	PRO	A	295	13.757	19.301	20.023	1.00	24.62
734	O	PRO	A	295	14.985	19.321	19.906	1.00	25.02
735	N	GLY	A	296	13.114	19.889	21.029	1.00	23.49
736	CA	GLY	A	296	13.854	20.563	22.081	1.00	23.80
737	C	GLY	A	296	14.022	22.064	21.948	1.00	22.79
738	O	GLY	A	296	14.240	22.752	22.948	1.00	21.27
739	N	PHE	A	297	13.928	22.583	20.728	1.00	22.01
740	CA	PHE	A	297	14.097	24.019	20.518	1.00	22.24
741	CB	PHE	A	297	14.011	24.358	19.025	1.00	21.13
742	CG	PHE	A	297	14.296	25.805	18.715	1.00	20.73
743	CD1	PHE	A	297	13.287	26.760	18.780	1.00	21.28
744	CD2	PHE	A	297	15.584	26.215	18.389	1.00	20.25
745	CE1	PHE	A	297	13.560	28.105	18.523	1.00	20.90
746	CE2	PHE	A	297	15.867	27.556	18.131	1.00	19.14
747	CZ	PHE	A	297	14.856	28.500	18.199	1.00	19.75
748	C	PHE	A	297	13.080	24.854	21.289	1.00	22.26
749	O	PHE	A	297	13.439	25.835	21.945	1.00	22.51
750	N	ALA	A	298	11.813	24.464	21.217	1.00	23.86
751	CA	ALA	A	298	10.754	25.206	21.896	1.00	24.65
752	CB	ALA	A	298	9.391	24.693	21.450	1.00	25.58

753	C	ALA	A	298	10.862	25.154	23.418	1.00	25.96
754	O	ALA	A	298	10.229	25.947	24.111	1.00	26.50
755	N	ASN	A	299	11.668	24.230	23.933	1.00	26.32
756	CA	ASN	A	299	11.856	24.088	25.377	1.00	26.91
757	CB	ASN	A	299	12.296	22.663	25.714	1.00	27.32
758	CG	ASN	A	299	11.198	21.648	25.496	1.00	27.93
759	OD1	ASN	A	299	11.456	20.447	25.428	1.00	31.25
760	ND2	ASN	A	299	9.962	22.123	25.393	1.00	27.97
761	C	ASN	A	299	12.891	25.068	25.923	1.00	27.12
762	O	ASN	A	299	12.982	25.288	27.134	1.00	26.42
763	N	LEU	A	300	13.684	25.642	25.028	1.00	24.59
764	CA	LEU	A	300	14.705	26.596	25.433	1.00	23.00
765	CB	LEU	A	300	15.620	26.921	24.252	1.00	20.53
766	CG	LEU	A	300	16.484	25.795	23.687	1.00	20.80
767	CD1	LEU	A	300	17.176	26.283	22.424	1.00	20.69
768	CD2	LEU	A	300	17.509	25.357	24.729	1.00	21.60
769	C	LEU	A	300	14.046	27.873	25.909	1.00	21.59
770	O	LEU	A	300	12.900	28.141	25.571	1.00	20.49
771	N	ASP	A	301	14.771	28.654	26.703	1.00	23.45
772	CA	ASP	A	301	14.252	29.931	27.172	1.00	23.40
773	CB	ASP	A	301	15.276	30.636	28.058	1.00	22.34
774	CG	ASP	A	301	14.863	32.052	28.406	1.00	23.70
775	OD1	ASP	A	301	13.868	32.225	29.135	1.00	24.73
776	OD2	ASP	A	301	15.531	33.000	27.941	1.00	24.97
777	C	ASP	A	301	14.049	30.738	25.894	1.00	23.49
778	O	ASP	A	301	14.817	30.584	24.945	1.00	22.64
779	N	LEU	A	302	13.029	31.588	25.863	1.00	24.03
780	CA	LEU	A	302	12.760	32.376	24.665	1.00	24.61
781	CB	LEU	A	302	11.486	33.209	24.845	1.00	25.91
782	CG	LEU	A	302	11.303	34.143	26.039	1.00	29.90
783	CD1	LEU	A	302	12.353	35.243	26.046	1.00	31.19
784	CD2	LEU	A	302	9.910	34.751	25.944	1.00	32.22
785	C	LEU	A	302	13.914	33.274	24.222	1.00	23.78

786	O	LEU	A	302	14.078	33.525	23.031	1.00	22.46
787	N	ASN	A	303	14.710	33.764	25.168	1.00	22.87
788	CA	ASN	A	303	15.842	34.615	24.814	1.00	23.57
789	CB	ASN	A	303	16.499	35.183	26.072	1.00	24.41
790	CG	ASN	A	303	15.597	36.151	26.812	1.00	25.82
791	OD1	ASN	A	303	15.341	37.265	26.346	1.00	24.76
792	ND2	ASN	A	303	15.097	35.724	27.969	1.00	25.85
793	C	ASN	A	303	16.858	33.792	24.025	1.00	23.03
794	O	ASN	A	303	17.475	34.279	23.071	1.00	22.95
795	N	ASP	A	304	17.031	32.539	24.428	1.00	21.92
796	CA	ASP	A	304	17.965	31.659	23.742	1.00	21.37
797	CB	ASP	A	304	18.232	30.404	24.570	1.00	20.90
798	CG	ASP	A	304	19.282	30.630	25.640	1.00	20.90
799	OD1	ASP	A	304	19.790	31.766	25.753	1.00	22.16
800	OD2	ASP	A	304	19.602	29.671	26.365	1.00	22.62
801	C	ASP	A	304	17.414	31.284	22.375	1.00	20.42
802	O	ASP	A	304	18.177	31.074	21.433	1.00	21.27
803	N	GLN	A	305	16.091	31.200	22.264	1.00	19.98
804	CA	GLN	A	305	15.478	30.871	20.978	1.00	20.73
805	CB	GLN	A	305	13.969	30.644	21.124	1.00	20.41
806	CG	GLN	A	305	13.593	29.369	21.870	1.00	22.80
807	CD	GLN	A	305	12.093	29.135	21.911	1.00	24.47
808	OE1	GLN	A	305	11.420	29.157	20.880	1.00	26.99
809	NE2	GLN	A	305	11.562	28.903	23.107	1.00	23.97
810	C	GLN	A	305	15.738	32.036	20.027	1.00	19.47
811	O	GLN	A	305	16.093	31.838	18.865	1.00	19.20
812	N	VAL	A	306	15.561	33.250	20.539	1.00	19.92
813	CA	VAL	A	306	15.787	34.463	19.760	1.00	18.92
814	CB	VAL	A	306	15.414	35.717	20.582	1.00	19.64
815	CG1	VAL	A	306	15.853	36.982	19.860	1.00	20.62
816	CG2	VAL	A	306	13.912	35.747	20.802	1.00	19.50
817	C	VAL	A	306	17.246	34.559	19.321	1.00	18.13
818	O	VAL	A	306	17.539	34.860	18.160	1.00	17.71

819	N	THR	A	307	18.159	34.293	20.250	1.00	17.09
820	CA	THR	A	307	19.586	34.361	19.957	1.00	17.05
821	CB	THR	A	307	20.424	34.138	21.242	1.00	17.63
822	OG1	THR	A	307	20.153	35.197	22.171	1.00	16.06
823	CG2	THR	A	307	21.918	34.135	20.921	1.00	16.45
824	C	THR	A	307	20.006	33.346	18.892	1.00	16.61
825	O	THR	A	307	20.766	33.672	17.986	1.00	17.34
826	N	LEU	A	308	19.503	32.121	18.994	1.00	15.88
827	CA	LEU	A	308	19.865	31.093	18.025	1.00	16.20
828	CB	LEU	A	308	19.262	29.741	18.417	1.00	17.78
829	CG	LEU	A	308	19.884	29.111	19.664	1.00	16.63
830	CD1	LEU	A	308	19.285	27.720	19.912	1.00	17.89
831	CD2	LEU	A	308	21.393	29.016	19.472	1.00	17.96
832	C	LEU	A	308	19.422	31.479	16.622	1.00	16.44
833	O	LEU	A	308	20.154	31.263	15.650	1.00	17.08
834	N	LEU	A	309	18.224	32.043	16.511	1.00	16.59
835	CA	LEU	A	309	17.724	32.463	15.204	1.00	17.03
836	CB	LEU	A	309	16.211	32.710	15.261	1.00	16.97
837	CG	LEU	A	309	15.373	31.426	15.326	1.00	18.35
838	CD1	LEU	A	309	13.914	31.777	15.589	1.00	23.00
839	CD2	LEU	A	309	15.506	30.657	14.020	1.00	19.92
840	C	LEU	A	309	18.447	33.726	14.751	1.00	17.00
841	O	LEU	A	309	18.825	33.855	13.587	1.00	17.06
842	N	LYS	A	310	18.649	34.657	15.675	1.00	16.85
843	CA	LYS	A	310	19.332	35.903	15.336	1.00	17.88
844	CB	LYS	A	310	19.570	36.737	16.595	1.00	19.60
845	CG	LYS	A	310	20.250	38.079	16.325	1.00	21.39
846	CD	LYS	A	310	20.640	38.760	17.633	1.00	24.10
847	CE	LYS	A	310	21.273	40.120	17.385	1.00	24.44
848	NZ	LYS	A	310	20.305	41.066	16.750	1.00	26.22
849	C	LYS	A	310	20.670	35.659	14.632	1.00	18.39
850	O	LYS	A	310	20.956	36.276	13.605	1.00	19.24
851	N	TYR	A	311	21.478	34.751	15.174	1.00	16.44

852	CA	TYR	A	311	22.788	34.459	14.601	1.00	19.84
853	CB	TYR	A	311	23.784	34.136	15.719	1.00	23.67
854	CG	TYR	A	311	24.144	35.333	16.568	1.00	27.71
855	CD1	TYR	A	311	24.994	36.325	16.083	1.00	30.38
856	CE1	TYR	A	311	25.315	37.439	16.856	1.00	32.19
857	CD2	TYR	A	311	23.620	35.484	17.850	1.00	30.97
858	CE2	TYR	A	311	23.933	36.595	18.631	1.00	33.09
859	CZ	TYR	A	311	24.782	37.566	18.127	1.00	33.75
860	OH	TYR	A	311	25.107	38.659	18.895	1.00	36.85
861	C	TYR	A	311	22.803	33.336	13.573	1.00	17.92
862	O	TYR	A	311	23.712	33.261	12.743	1.00	20.86
863	N	GLY	A	312	21.799	32.469	13.610	1.00	16.75
864	CA	GLY	A	312	21.784	31.364	12.669	1.00	15.82
865	C	GLY	A	312	20.979	31.509	11.390	1.00	16.03
866	O	GLY	A	312	21.278	30.834	10.403	1.00	16.07
867	N	VAL	A	313	19.971	32.377	11.372	1.00	15.36
868	CA	VAL	A	313	19.154	32.494	10.170	1.00	16.30
869	CB	VAL	A	313	17.975	33.506	10.353	1.00	17.29
870	CG1	VAL	A	313	18.485	34.904	10.609	1.00	16.70
871	CG2	VAL	A	313	17.093	33.486	9.124	1.00	23.41
872	C	VAL	A	313	19.901	32.811	8.878	1.00	14.96
873	O	VAL	A	313	19.631	32.198	7.846	1.00	12.97
874	N	TYR	A	314	20.852	33.738	8.902	1.00	13.63
875	CA	TYR	A	314	21.539	34.047	7.654	1.00	14.50
876	CB	TYR	A	314	22.206	35.429	7.729	1.00	15.24
877	CG	TYR	A	314	21.201	36.518	7.423	1.00	15.95
878	CD1	TYR	A	314	20.785	36.754	6.115	1.00	16.47
879	CE1	TYR	A	314	19.764	37.664	5.838	1.00	17.10
880	CD2	TYR	A	314	20.578	37.230	8.452	1.00	15.91
881	CE2	TYR	A	314	19.563	38.137	8.190	1.00	15.61
882	CZ	TYR	A	314	19.156	38.349	6.883	1.00	16.58
883	OH	TYR	A	314	18.128	39.229	6.619	1.00	17.94
884	C	TYR	A	314	22.514	32.968	7.212	1.00	14.15

885	O	TYR	A	314	22.786	32.827	6.017	1.00	14.15
886	N	GLU	A	315	23.041	32.198	8.159	1.00	12.79
887	CA	GLU	A	315	23.939	31.113	7.776	1.00	13.63
888	CB	GLU	A	315	24.581	30.471	9.012	1.00	15.05
889	CG	GLU	A	315	25.608	31.379	9.701	1.00	15.42
890	CD	GLU	A	315	26.281	30.734	10.900	1.00	16.70
891	OE1	GLU	A	315	26.093	29.520	11.125	1.00	17.95
892	OE2	GLU	A	315	27.008	31.446	11.617	1.00	16.57
893	C	GLU	A	315	23.055	30.102	7.034	1.00	14.04
894	O	GLU	A	315	23.449	29.549	6.007	1.00	12.76
895	N	ALA	A	316	21.842	29.895	7.545	1.00	13.17
896	CA	ALA	A	316	20.906	28.953	6.930	1.00	13.03
897	CB	ALA	A	316	19.701	28.721	7.846	1.00	13.75
898	C	ALA	A	316	20.435	29.488	5.589	1.00	13.24
899	O	ALA	A	316	20.327	28.748	4.612	1.00	12.79
900	N	ILE	A	317	20.146	30.784	5.544	1.00	12.44
901	CA	ILE	A	317	19.693	31.399	4.306	1.00	11.19
902	CB	ILE	A	317	19.360	32.896	4.534	1.00	10.99
903	CG2	ILE	A	317	19.215	33.639	3.193	1.00	11.43
904	CG1	ILE	A	317	18.053	32.999	5.325	1.00	12.81
905	CD1	ILE	A	317	17.711	34.415	5.775	1.00	13.13
906	C	ILE	A	317	20.720	31.242	3.184	1.00	12.02
907	O	ILE	A	317	20.377	30.815	2.082	1.00	12.18
908	N	PHE	A	318	21.980	31.566	3.450	1.00	13.30
909	CA	PHE	A	318	22.982	31.429	2.393	1.00	13.60
910	CB	PHE	A	318	24.275	32.137	2.797	1.00	14.04
911	CG	PHE	A	318	24.095	33.610	3.056	1.00	13.96
912	CD1	PHE	A	318	23.204	34.355	2.287	1.00	16.84
913	CD2	PHE	A	318	24.815	34.252	4.056	1.00	15.29
914	CE1	PHE	A	318	23.030	35.722	2.509	1.00	17.71
915	CE2	PHE	A	318	24.649	35.616	4.285	1.00	18.04
916	CZ	PHE	A	318	23.750	36.350	3.506	1.00	15.92
917	C	PHE	A	318	23.233	29.959	2.024	1.00	13.74

918	O	PHE	A	318	23.540	29.647	0.875	1.00	13.80
919	N	ALA	A	319	23.103	29.054	2.989	1.00	13.03
920	CA	ALA	A	319	23.275	27.631	2.698	1.00	12.43
921	CB	ALA	A	319	23.257	26.807	4.001	1.00	11.53
922	C	ALA	A	319	22.127	27.186	1.781	1.00	13.70
923	O	ALA	A	319	22.340	26.474	0.792	1.00	13.68
924	N	MET	A	320	20.906	27.612	2.102	1.00	12.83
925	CA	MET	A	320	19.754	27.229	1.291	1.00	11.87
926	CB	MET	A	320	18.446	27.436	2.071	1.00	14.42
927	CG	MET	A	320	18.375	26.587	3.347	1.00	16.28
928	SD	MET	A	320	16.760	26.610	4.149	1.00	18.54
929	CE	MET	A	320	16.612	28.349	4.548	1.00	20.41
930	C	MET	A	320	19.690	27.941	-0.060	1.00	13.87
931	O	MET	A	320	19.023	27.464	-0.976	1.00	12.13
932	N	LEU	A	321	20.376	29.077	-0.197	1.00	13.97
933	CA	LEU	A	321	20.371	29.775	-1.485	1.00	15.41
934	CB	LEU	A	321	21.223	31.051	-1.424	1.00	15.37
935	CG	LEU	A	321	20.547	32.292	-0.829	1.00	18.20
936	CD1	LEU	A	321	21.490	33.490	-0.942	1.00	19.32
937	CD2	LEU	A	321	19.231	32.569	-1.561	1.00	18.93
938	C	LEU	A	321	20.935	28.854	-2.560	1.00	13.60
939	O	LEU	A	321	20.499	28.874	-3.712	1.00	15.79
940	N	SER	A	322	21.919	28.052	-2.168	1.00	12.99
941	CA	SER	A	322	22.575	27.121	-3.072	1.00	14.61
942	CB	SER	A	322	23.541	26.240	-2.276	1.00	14.55
943	OG	SER	A	322	24.372	27.042	-1.457	1.00	15.05
944	C	SER	A	322	21.552	26.244	-3.797	1.00	15.16
945	O	SER	A	322	21.734	25.892	-4.963	1.00	16.58
946	N	SER	A	323	20.476	25.899	-3.099	1.00	14.05
947	CA	SER	A	323	19.439	25.051	-3.675	1.00	14.37
948	CB	SER	A	323	18.390	24.708	-2.615	1.00	16.17
949	OG	SER	A	323	18.989	24.036	-1.524	1.00	14.97
950	C	SER	A	323	18.741	25.667	-4.883	1.00	15.39

951	O	SER	A	323	18.260	24.947	-5.759	1.00	15.48
952	N	VAL	A	324	18.672	26.995	-4.927	1.00	16.08
953	CA	VAL	A	324	17.999	27.667	-6.029	1.00	16.93
954	CB	VAL	A	324	16.974	28.713	-5.516	1.00	18.06
955	CG1	VAL	A	324	15.878	28.020	-4.716	1.00	20.27
956	CG2	VAL	A	324	17.674	29.766	-4.667	1.00	19.05
957	C	VAL	A	324	18.967	28.358	-6.973	1.00	16.26
958	O	VAL	A	324	18.551	29.150	-7.816	1.00	17.98
959	N	MET	A	325	20.251	28.034	-6.853	1.00	16.16
960	CA	MET	A	325	21.276	28.648	-7.700	1.00	17.20
961	CB	MET	A	325	22.355	29.329	-6.846	1.00	16.55
962	CG	MET	A	325	21.941	30.527	-6.005	1.00	16.51
963	SD	MET	A	325	23.361	31.079	-4.984	1.00	17.83
964	CE	MET	A	325	22.982	32.821	-4.800	1.00	19.15
965	C	MET	A	325	22.021	27.664	-8.596	1.00	19.13
966	O	MET	A	325	22.098	26.470	-8.308	1.00	20.24
967	N	ASN	A	326	22.557	28.188	-9.694	1.00	19.31
968	CA	ASN	A	326	23.425	27.418	-10.572	1.00	20.10
969	CB	ASN	A	326	22.716	26.858	-11.821	1.00	21.23
970	CG	ASN	A	326	22.149	27.919	-12.730	1.00	20.10
971	OD1	ASN	A	326	22.672	29.028	-12.837	1.00	21.27
972	ND2	ASN	A	326	21.076	27.559	-13.434	1.00	23.09
973	C	ASN	A	326	24.498	28.453	-10.909	1.00	21.45
974	O	ASN	A	326	24.426	29.580	-10.423	1.00	19.65
975	N	LYS	A	327	25.488	28.098	-11.717	1.00	21.83
976	CA	LYS	A	327	26.560	29.043	-12.011	1.00	23.64
977	CB	LYS	A	327	27.655	28.364	-12.841	1.00	26.31
978	CG	LYS	A	327	27.285	28.119	-14.297	1.00	30.33
979	CD	LYS	A	327	28.506	27.647	-15.083	1.00	34.09
980	CE	LYS	A	327	28.258	27.640	-16.589	1.00	36.35
981	NZ	LYS	A	327	27.208	26.665	-16.992	1.00	39.18
982	C	LYS	A	327	26.158	30.342	-12.704	1.00	22.90
983	O	LYS	A	327	26.924	31.308	-12.685	1.00	22.33

984	N	ASP	A	328	24.965	30.387	-13.290	1.00	21.50
985	CA	ASP	A	328	24.544	31.582	-14.020	1.00	21.46
986	CB	ASP	A	328	24.110	31.185	-15.433	1.00	22.79
987	CG	ASP	A	328	25.228	30.535	-16.219	1.00	24.81
988	OD1	ASP	A	328	26.327	31.124	-16.295	1.00	28.16
989	OD2	ASP	A	328	25.010	29.440	-16.760	1.00	26.38
990	C	ASP	A	328	23.462	32.463	-13.404	1.00	19.81
991	O	ASP	A	328	23.123	33.505	-13.967	1.00	18.99
992	N	GLY	A	329	22.915	32.061	-12.263	1.00	18.40
993	CA	GLY	A	329	21.879	32.872	-11.648	1.00	17.35
994	C	GLY	A	329	21.093	32.134	-10.584	1.00	16.28
995	O	GLY	A	329	21.466	31.030	-10.186	1.00	15.47
996	N	MET	A	330	20.002	32.739	-10.120	1.00	17.05
997	CA	MET	A	330	19.183	32.109	-9.089	1.00	17.55
998	CB	MET	A	330	19.563	32.642	-7.701	1.00	19.90
999	CG	MET	A	330	19.221	34.098	-7.438	1.00	22.04
1000	SD	MET	A	330	19.415	34.525	-5.667	1.00	24.36
1001	CE	MET	A	330	17.856	34.142	-5.014	1.00	23.38
1002	C	MET	A	330	17.689	32.295	-9.308	1.00	17.11
1003	O	MET	A	330	17.249	33.259	-9.930	1.00	17.45
1004	N	LEU	A	331	16.908	31.350	-8.799	1.00	16.64
1005	CA	LEU	A	331	15.460	31.411	-8.912	1.00	16.30
1006	CB	LEU	A	331	14.843	30.051	-8.595	1.00	17.42
1007	CG	LEU	A	331	15.026	28.943	-9.620	1.00	19.04
1008	CD1	LEU	A	331	14.408	27.650	-9.079	1.00	18.84
1009	CD2	LEU	A	331	14.363	29.359	-10.925	1.00	17.82
1010	C	LEU	A	331	14.930	32.414	-7.903	1.00	16.49
1011	O	LEU	A	331	15.415	32.465	-6.774	1.00	17.61
1012	N	VAL	A	332	13.932	33.194	-8.305	1.00	14.86
1013	CA	VAL	A	332	13.331	34.173	-7.409	1.00	15.11
1014	CB	VAL	A	332	13.880	35.603	-7.664	1.00	14.89
1015	CG1	VAL	A	332	15.406	35.600	-7.537	1.00	17.85
1016	CG2	VAL	A	332	13.453	36.099	-9.040	1.00	16.47

1017	C	VAL	A	332	11.821	34.193	-7.589	1.00	14.36
1018	O	VAL	A	332	11.283	33.559	-8.501	1.00	15.87
1019	N	ALA	A	333	11.148	34.928	-6.713	1.00	13.97
1020	CA	ALA	A	333	9.698	35.071	-6.757	1.00	14.91
1021	CB	ALA	A	333	9.294	35.898	-7.977	1.00	15.58
1022	C	ALA	A	333	8.978	33.724	-6.768	1.00	14.63
1023	O	ALA	A	333	8.168	33.441	-7.660	1.00	14.60
1024	N	TYR	A	334	9.285	32.899	-5.772	1.00	14.26
1025	CA	TYR	A	334	8.660	31.589	-5.630	1.00	15.27
1026	CB	TYR	A	334	7.195	31.781	-5.230	1.00	15.76
1027	CG	TYR	A	334	7.086	32.362	-3.840	1.00	18.04
1028	CD1	TYR	A	334	7.025	31.532	-2.722	1.00	19.51
1029	CE1	TYR	A	334	7.073	32.055	-1.432	1.00	20.29
1030	CD2	TYR	A	334	7.182	33.737	-3.634	1.00	19.02
1031	CE2	TYR	A	334	7.237	34.272	-2.348	1.00	20.93
1032	CZ	TYR	A	334	7.186	33.427	-1.253	1.00	20.76
1033	OH	TYR	A	334	7.284	33.950	0.019	1.00	21.61
1034	C	TYR	A	334	8.797	30.715	-6.871	1.00	14.54
1035	O	TYR	A	334	7.854	30.038	-7.290	1.00	15.22
1036	N	GLY	A	335	9.996	30.744	-7.441	1.00	15.09
1037	CA	GLY	A	335	10.306	29.944	-8.612	1.00	16.73
1038	C	GLY	A	335	9.795	30.441	-9.946	1.00	18.37
1039	O	GLY	A	335	9.965	29.761	-10.958	1.00	18.69
1040	N	ASN	A	336	9.188	31.623	-9.972	1.00	18.57
1041	CA	ASN	A	336	8.654	32.133	-11.227	1.00	18.81
1042	CB	ASN	A	336	7.322	32.835	-10.988	1.00	21.87
1043	CG	ASN	A	336	6.149	31.866	-10.981	1.00	24.72
1044	OD1	ASN	A	336	5.003	32.275	-10.900	1.00	32.52
1045	ND2	ASN	A	336	6.437	30.579	-11.071	1.00	29.15
1046	C	ASN	A	336	9.595	33.053	-11.993	1.00	18.54
1047	O	ASN	A	336	9.277	33.492	-13.096	1.00	16.73
1048	N	GLY	A	337	10.749	33.335	-11.406	1.00	16.20
1049	CA	GLY	A	337	11.717	34.187	-12.066	1.00	16.52

1050	C	GLY	A	337	13.114	33.638	-11.886	1.00	16.47
1051	O	GLY	A	337	13.347	32.809	-11.008	1.00	15.40
1052	N	PHE	A	338	14.041	34.090	-12.728	1.00	15.82
1053	CA	PHE	A	338	15.436	33.672	-12.654	1.00	15.40
1054	CB	PHE	A	338	15.722	32.543	-13.651	1.00	16.65
1055	CG	PHE	A	338	17.156	32.066	-13.641	1.00	20.70
1056	CD1	PHE	A	338	18.113	32.664	-14.464	1.00	19.82
1057	CD2	PHE	A	338	17.548	31.021	-12.808	1.00	19.54
1058	CE1	PHE	A	338	19.433	32.225	-14.460	1.00	22.34
1059	CE2	PHE	A	338	18.873	30.570	-12.794	1.00	22.09
1060	CZ	PHE	A	338	19.816	31.174	-13.624	1.00	22.09
1061	C	PHE	A	338	16.265	34.904	-12.994	1.00	16.41
1062	O	PHE	A	338	16.212	35.411	-14.117	1.00	15.80
1063	N	ILE	A	339	17.014	35.397	-12.015	1.00	14.27
1064	CA	ILE	A	339	17.828	36.581	-12.229	1.00	15.49
1065	CB	ILE	A	339	17.689	37.550	-11.028	1.00	15.76
1066	CG2	ILE	A	339	18.192	36.892	-9.760	1.00	17.30
1067	CG1	ILE	A	339	18.434	38.853	-11.311	1.00	15.24
1068	CD1	ILE	A	339	17.955	39.999	-10.429	1.00	16.30
1069	C	ILE	A	339	19.274	36.151	-12.453	1.00	16.57
1070	O	ILE	A	339	19.835	35.379	-11.676	1.00	16.99
1071	N	THR	A	340	19.884	36.644	-13.526	1.00	15.69
1072	CA	THR	A	340	21.251	36.232	-13.835	1.00	17.54
1073	CB	THR	A	340	21.625	36.501	-15.321	1.00	18.08
1074	OG1	THR	A	340	21.680	37.913	-15.563	1.00	18.08
1075	CG2	THR	A	340	20.611	35.876	-16.239	1.00	19.40
1076	C	THR	A	340	22.337	36.840	-12.973	1.00	17.79
1077	O	THR	A	340	22.272	38.001	-12.551	1.00	17.03
1078	N	ARG	A	341	23.347	36.019	-12.729	1.00	18.29
1079	CA	ARG	A	341	24.503	36.395	-11.944	1.00	20.41
1080	CB	ARG	A	341	25.470	35.216	-11.910	1.00	20.86
1081	CG	ARG	A	341	26.710	35.443	-11.093	1.00	23.49
1082	CD	ARG	A	341	27.502	34.152	-11.003	1.00	22.29

1083	NE	ARG	A	341	28.625	34.282	-10.089	1.00	25.39
1084	CZ	ARG	A	341	29.432	33.283	-9.755	1.00	25.74
1085	NH1	ARG	A	341	29.239	32.074	-10.264	1.00	25.82
1086	NH2	ARG	A	341	30.427	33.495	-8.908	1.00	25.63
1087	C	ARG	A	341	25.175	37.606	-12.587	1.00	20.85
1088	O	ARG	A	341	25.630	38.515	-11.900	1.00	20.39
1089	N	GLU	A	342	25.225	37.615	-13.915	1.00	21.71
1090	CA	GLU	A	342	25.858	38.717	-14.633	1.00	23.42
1091	CB	GLU	A	342	26.044	38.343	-16.104	1.00	26.93
1092	CG	GLU	A	342	27.151	37.324	-16.330	1.00	31.26
1093	CD	GLU	A	342	28.501	37.816	-15.832	1.00	33.51
1094	OE1	GLU	A	342	28.961	38.882	-16.294	1.00	36.23
1095	OE2	GLU	A	342	29.105	37.140	-14.977	1.00	36.72
1096	C	GLU	A	342	25.101	40.037	-14.510	1.00	21.78
1097	O	GLU	A	342	25.715	41.103	-14.425	1.00	23.51
1098	N	PHE	A	343	23.774	39.974	-14.496	1.00	20.79
1099	CA	PHE	A	343	22.982	41.188	-14.358	1.00	20.13
1100	CB	PHE	A	343	21.491	40.880	-14.534	1.00	21.21
1101	CG	PHE	A	343	20.598	42.065	-14.304	1.00	22.31
1102	CD1	PHE	A	343	20.800	43.255	-15.003	1.00	22.58
1103	CD2	PHE	A	343	19.556	41.998	-13.385	1.00	22.12
1104	CE1	PHE	A	343	19.978	44.356	-14.784	1.00	22.50
1105	CE2	PHE	A	343	18.729	43.095	-13.159	1.00	21.07
1106	CZ	PHE	A	343	18.940	44.277	-13.861	1.00	23.38
1107	C	PHE	A	343	23.237	41.787	-12.973	1.00	20.06
1108	O	PHE	A	343	23.389	42.998	-12.821	1.00	18.10
1109	N	LEU	A	344	23.291	40.929	-11.959	1.00	19.09
1110	CA	LEU	A	344	23.535	41.390	-10.599	1.00	19.98
1111	CB	LEU	A	344	23.434	40.211	-9.629	1.00	18.81
1112	CG	LEU	A	344	22.003	39.699	-9.449	1.00	17.36
1113	CD1	LEU	A	344	22.030	38.298	-8.865	1.00	17.66
1114	CD2	LEU	A	344	21.222	40.668	-8.541	1.00	18.64
1115	C	LEU	A	344	24.891	42.082	-10.451	1.00	20.25

1116	O	LEU	A	344	25.000	43.113	-9.785	1.00	20.17
1117	N	LYS	A	345	25.926	41.532	-11.077	1.00	22.58
1118	CA	LYS	A	345	27.243	42.149	-10.976	1.00	25.12
1119	CB	LYS	A	345	28.329	41.149	-11.388	1.00	28.30
1120	CG	LYS	A	345	28.086	40.453	-12.709	1.00	31.49
1121	CD	LYS	A	345	28.931	39.185	-12.824	1.00	34.20
1122	CE	LYS	A	345	30.418	39.474	-12.663	1.00	32.93
1123	NZ	LYS	A	345	31.242	38.267	-12.935	1.00	33.54
1124	C	LYS	A	345	27.349	43.442	-11.787	1.00	26.38
1125	O	LYS	A	345	28.246	44.259	-11.551	1.00	28.05
1126	N	SER	A	346	26.411	43.644	-12.713	1.00	25.99
1127	CA	SER	A	346	26.397	44.840	-13.557	1.00	25.78
1128	CB	SER	A	346	25.596	44.590	-14.834	1.00	27.38
1129	OG	SER	A	346	24.206	44.742	-14.590	1.00	27.61
1130	C	SER	A	346	25.782	46.028	-12.832	1.00	25.54
1131	O	SER	A	346	25.870	47.169	-13.298	1.00	24.80
1132	N	LEU	A	347	25.151	45.762	-11.694	1.00	21.74
1133	CA	LEU	A	347	24.529	46.826	-10.925	1.00	21.47
1134	CB	LEU	A	347	23.686	46.242	-9.790	1.00	20.68
1135	CG	LEU	A	347	22.544	45.312	-10.207	1.00	17.94
1136	CD1	LEU	A	347	21.932	44.695	-8.952	1.00	17.43
1137	CD2	LEU	A	347	21.497	46.094	-10.998	1.00	18.91
1138	C	LEU	A	347	25.585	47.751	-10.341	1.00	22.34
1139	O	LEU	A	347	26.773	47.431	-10.306	1.00	21.32
1140	N	ARG	A	348	25.133	48.904	-9.878	1.00	23.03
1141	CA	ARG	A	348	26.007	49.899	-9.279	1.00	24.90
1142	CB	ARG	A	348	25.247	51.233	-9.226	1.00	26.16
1143	CG	ARG	A	348	25.445	52.062	-7.977	1.00	28.63
1144	CD	ARG	A	348	24.782	53.424	-8.123	1.00	27.93
1145	NE	ARG	A	348	23.514	53.557	-7.407	1.00	25.84
1146	CZ	ARG	A	348	23.385	53.485	-6.086	1.00	25.53
1147	NH1	ARG	A	348	24.446	53.264	-5.318	1.00	26.92
1148	NH2	ARG	A	348	22.201	53.676	-5.526	1.00	26.63

1149	C	ARG	A	348	26.431	49.457	-7.877	1.00	23.21
1150	O	ARG	A	348	25.666	48.796	-7.177	1.00	22.61
1151	N	LYS	A	349	27.654	49.799	-7.472	1.00	23.12
1152	CA	LYS	A	349	28.104	49.457	-6.126	1.00	22.49
1153	CB	LYS	A	349	29.575	49.848	-5.910	1.00	23.58
1154	CG	LYS	A	349	30.585	49.055	-6.738	1.00	22.91
1155	CD	LYS	A	349	32.017	49.580	-6.540	1.00	25.76
1156	CE	LYS	A	349	32.665	49.069	-5.261	1.00	26.68
1157	NZ	LYS	A	349	33.144	47.662	-5.407	1.00	28.29
1158	C	LYS	A	349	27.218	50.268	-5.188	1.00	22.76
1159	O	LYS	A	349	26.765	51.361	-5.545	1.00	24.51
1160	N	PRO	A	350	26.975	49.767	-3.970	1.00	21.69
1161	CD	PRO	A	350	26.248	50.523	-2.935	1.00	23.55
1162	CA	PRO	A	350	27.476	48.506	-3.421	1.00	21.20
1163	CB	PRO	A	350	27.573	48.818	-1.943	1.00	23.13
1164	CG	PRO	A	350	26.312	49.586	-1.724	1.00	22.88
1165	C	PRO	A	350	26.544	47.322	-3.685	1.00	20.65
1166	O	PRO	A	350	26.815	46.197	-3.256	1.00	20.59
1167	N	PHE	A	351	25.447	47.576	-4.387	1.00	19.16
1168	CA	PHE	A	351	24.475	46.525	-4.666	1.00	18.85
1169	CB	PHE	A	351	23.252	47.140	-5.349	1.00	20.28
1170	CG	PHE	A	351	22.539	48.141	-4.487	1.00	19.94
1171	CD1	PHE	A	351	21.737	47.720	-3.427	1.00	18.19
1172	CD2	PHE	A	351	22.720	49.507	-4.690	1.00	18.89
1173	CE1	PHE	A	351	21.125	48.645	-2.576	1.00	19.37
1174	CE2	PHE	A	351	22.115	50.436	-3.848	1.00	19.54
1175	CZ	PHE	A	351	21.316	50.005	-2.786	1.00	19.87
1176	C	PHE	A	351	25.040	45.361	-5.469	1.00	19.99
1177	O	PHE	A	351	24.620	44.213	-5.289	1.00	19.11
1178	N	CYS	A	352	26.011	45.642	-6.334	1.00	17.57
1179	CA	CYS	A	352	26.622	44.589	-7.138	1.00	18.30
1180	CB	CYS	A	352	27.358	45.197	-8.335	1.00	18.99
1181	SG	CYS	A	352	28.659	46.372	-7.868	1.00	20.67

1182	C	CYS	A	352	27.599	43.760	-6.307	1.00	18.14
1183	O	CYS	A	352	28.107	42.743	-6.772	1.00	17.82
1184	N	ASP	A	353	27.843	44.184	-5.069	1.00	18.21
1185	CA	ASP	A	353	28.781	43.477	-4.206	1.00	18.60
1186	CB	ASP	A	353	29.640	44.484	-3.439	1.00	20.06
1187	CG	ASP	A	353	30.432	45.395	-4.364	1.00	20.29
1188	OD1	ASP	A	353	31.032	44.880	-5.319	1.00	21.00
1189	OD2	ASP	A	353	30.457	46.621	-4.137	1.00	22.31
1190	C	ASP	A	353	28.109	42.533	-3.223	1.00	19.14
1191	O	ASP	A	353	28.771	41.917	-2.386	1.00	20.18
1192	N	ILE	A	354	26.794	42.410	-3.340	1.00	17.15
1193	CA	ILE	A	354	26.023	41.562	-2.445	1.00	18.64
1194	CB	ILE	A	354	24.539	42.001	-2.422	1.00	19.28
1195	CG2	ILE	A	354	23.727	41.075	-1.521	1.00	17.16
1196	CG1	ILE	A	354	24.431	43.451	-1.940	1.00	19.43
1197	CD1	ILE	A	354	23.014	43.997	-1.956	1.00	19.79
1198	C	ILE	A	354	26.042	40.074	-2.778	1.00	18.41
1199	O	ILE	A	354	26.427	39.245	-1.951	1.00	17.58
1200	N	MET	A	355	25.630	39.743	-3.996	1.00	20.04
1201	CA	MET	A	355	25.507	38.349	-4.406	1.00	18.56
1202	CB	MET	A	355	24.429	38.241	-5.490	1.00	19.49
1203	CG	MET	A	355	23.033	38.634	-5.014	1.00	20.24
1204	SD	MET	A	355	22.487	37.687	-3.565	1.00	20.20
1205	CE	MET	A	355	22.589	36.017	-4.219	1.00	16.96
1206	C	MET	A	355	26.702	37.497	-4.821	1.00	18.99
1207	O	MET	A	355	26.655	36.283	-4.637	1.00	17.53
1208	N	GLU	A	356	27.764	38.084	-5.373	1.00	19.55
1209	CA	GLU	A	356	28.904	37.265	-5.800	1.00	19.92
1210	CB	GLU	A	356	30.072	38.135	-6.292	1.00	21.97
1211	CG	GLU	A	356	30.017	38.502	-7.762	1.00	26.26
1212	CD	GLU	A	356	29.835	37.292	-8.663	1.00	27.30
1213	OE1	GLU	A	356	28.697	37.049	-9.107	1.00	26.68
1214	OE2	GLU	A	356	30.826	36.575	-8.920	1.00	29.91

1215	C	GLU	A	356	29.432	36.288	-4.752	1.00	18.52
1216	O	GLU	A	356	29.624	35.112	-5.046	1.00	18.23
1217	N	PRO	A	357	29.686	36.758	-3.522	1.00	18.98
1218	CD	PRO	A	357	29.538	38.130	-3.001	1.00	20.10
1219	CA	PRO	A	357	30.195	35.863	-2.477	1.00	19.09
1220	CB	PRO	A	357	30.290	36.777	-1.259	1.00	20.02
1221	CG	PRO	A	357	30.525	38.137	-1.869	1.00	20.53
1222	C	PRO	A	357	29.273	34.664	-2.217	1.00	17.84
1223	O	PRO	A	357	29.730	33.572	-1.869	1.00	15.96
1224	N	LYS	A	358	27.973	34.883	-2.379	1.00	17.85
1225	CA	LYS	A	358	26.984	33.832	-2.161	1.00	16.69
1226	CB	LYS	A	358	25.594	34.448	-1.963	1.00	17.55
1227	CG	LYS	A	358	25.399	35.180	-0.625	1.00	16.13
1228	CD	LYS	A	358	26.255	36.439	-0.520	1.00	18.57
1229	CE	LYS	A	358	25.812	37.337	0.632	1.00	16.06
1230	NZ	LYS	A	358	26.664	38.570	0.749	1.00	15.29
1231	C	LYS	A	358	26.961	32.848	-3.327	1.00	17.68
1232	O	LYS	A	358	26.787	31.638	-3.132	1.00	17.04
1233	N	PHE	A	359	27.122	33.359	-4.544	1.00	17.39
1234	CA	PHE	A	359	27.153	32.478	-5.709	1.00	16.62
1235	CB	PHE	A	359	27.167	33.290	-7.012	1.00	16.38
1236	CG	PHE	A	359	25.795	33.651	-7.523	1.00	18.08
1237	CD1	PHE	A	359	24.944	32.671	-8.037	1.00	17.39
1238	CD2	PHE	A	359	25.355	34.970	-7.497	1.00	16.89
1239	CE1	PHE	A	359	23.679	33.004	-8.514	1.00	17.41
1240	CE2	PHE	A	359	24.093	35.313	-7.970	1.00	16.42
1241	CZ	PHE	A	359	23.253	34.327	-8.481	1.00	16.76
1242	C	PHE	A	359	28.421	31.633	-5.598	1.00	16.15
1243	O	PHE	A	359	28.400	30.424	-5.851	1.00	16.24
1244	N	ASP	A	360	29.526	32.263	-5.201	1.00	18.27
1245	CA	ASP	A	360	30.777	31.519	-5.050	1.00	18.69
1246	CB	ASP	A	360	31.948	32.453	-4.710	1.00	20.51
1247	CG	ASP	A	360	32.445	33.229	-5.922	1.00	22.65

1248	OD1	ASP	A	360	32.334	32.705	-7.048	1.00	23.09
1249	OD2	ASP	A	360	32.958	34.354	-5.752	1.00	27.87
1250	C	ASP	A	360	30.637	30.432	-3.988	1.00	18.16
1251	O	ASP	A	360	31.115	29.311	-4.177	1.00	17.43
1252	N	PHE	A	361	29.975	30.745	-2.876	1.00	16.51
1253	CA	PHE	A	361	29.793	29.736	-1.838	1.00	17.11
1254	CB	PHE	A	361	29.160	30.326	-0.574	1.00	17.43
1255	CG	PHE	A	361	28.769	29.280	0.441	1.00	16.12
1256	CD1	PHE	A	361	27.557	28.600	0.328	1.00	15.11
1257	CD2	PHE	A	361	29.642	28.927	1.469	1.00	16.71
1258	CE1	PHE	A	361	27.219	27.580	1.223	1.00	14.11
1259	CE2	PHE	A	361	29.314	27.909	2.367	1.00	15.23
1260	CZ	PHE	A	361	28.101	27.235	2.242	1.00	11.27
1261	C	PHE	A	361	28.905	28.605	-2.347	1.00	16.98
1262	O	PHE	A	361	29.211	27.431	-2.147	1.00	16.87
1263	N	ALA	A	362	27.803	28.971	-2.994	1.00	16.32
1264	CA	ALA	A	362	26.851	27.993	-3.517	1.00	19.25
1265	CB	ALA	A	362	25.659	28.714	-4.145	1.00	17.22
1266	C	ALA	A	362	27.460	27.021	-4.528	1.00	19.60
1267	O	ALA	A	362	27.080	25.850	-4.579	1.00	20.69
1268	N	MET	A	363	28.396	27.502	-5.337	1.00	19.90
1269	CA	MET	A	363	29.021	26.649	-6.343	1.00	23.22
1270	CB	MET	A	363	29.940	27.473	-7.244	1.00	25.16
1271	CG	MET	A	363	29.601	27.362	-8.717	1.00	31.86
1272	SD	MET	A	363	27.851	27.659	-9.059	1.00	35.24
1273	CE	MET	A	363	27.233	25.996	-9.144	1.00	37.40
1274	C	MET	A	363	29.808	25.533	-5.672	1.00	22.48
1275	O	MET	A	363	29.718	24.373	-6.069	1.00	22.07
1276	N	LYS	A	364	30.576	25.884	-4.647	1.00	21.68
1277	CA	LYS	A	364	31.349	24.884	-3.932	1.00	22.55
1278	CB	LYS	A	364	32.446	25.564	-3.104	1.00	24.59
1279	CG	LYS	A	364	33.595	26.061	-3.982	1.00	28.52
1280	CD	LYS	A	364	34.721	26.718	-3.203	1.00	31.12

1281	CE	LYS	A	364	34.316	28.080	-2.674	1.00	33.08
1282	NZ	LYS	A	364	35.512	28.842	-2.220	1.00	34.91
1283	C	LYS	A	364	30.438	24.022	-3.056	1.00	22.72
1284	O	LYS	A	364	30.699	22.834	-2.861	1.00	22.63
1285	N	PHE	A	365	29.358	24.610	-2.547	1.00	21.24
1286	CA	PHE	A	365	28.429	23.855	-1.705	1.00	20.87
1287	CB	PHE	A	365	27.423	24.794	-1.027	1.00	19.09
1288	CG	PHE	A	365	26.652	24.151	0.098	1.00	19.22
1289	CD1	PHE	A	365	27.263	23.902	1.322	1.00	19.37
1290	CD2	PHE	A	365	25.311	23.807	-0.063	1.00	19.20
1291	CE1	PHE	A	365	26.547	23.321	2.376	1.00	18.07
1292	CE2	PHE	A	365	24.585	23.227	0.978	1.00	18.27
1293	CZ	PHE	A	365	25.204	22.984	2.202	1.00	18.45
1294	C	PHE	A	365	27.667	22.819	-2.532	1.00	20.34
1295	O	PHE	A	365	27.492	21.672	-2.106	1.00	19.46
1296	N	ASN	A	366	27.212	23.232	-3.712	1.00	20.08
1297	CA	ASN	A	366	26.463	22.354	-4.606	1.00	21.22
1298	CB	ASN	A	366	25.910	23.158	-5.789	1.00	21.85
1299	CG	ASN	A	366	24.619	23.893	-5.448	1.00	22.68
1300	OD1	ASN	A	366	24.237	24.853	-6.124	1.00	22.40
1301	ND2	ASN	A	366	23.935	23.434	-4.406	1.00	20.32
1302	C	ASN	A	366	27.324	21.202	-5.120	1.00	21.97
1303	O	ASN	A	366	26.806	20.147	-5.495	1.00	22.05
1304	N	ALA	A	367	28.636	21.409	-5.132	1.00	20.80
1305	CA	ALA	A	367	29.564	20.381	-5.587	1.00	22.52
1306	CB	ALA	A	367	30.977	20.942	-5.660	1.00	22.39
1307	C	ALA	A	367	29.519	19.188	-4.638	1.00	23.80
1308	O	ALA	A	367	30.003	18.102	-4.969	1.00	24.70
1309	N	LEU	A	368	28.942	19.395	-3.455	1.00	22.37
1310	CA	LEU	A	368	28.820	18.328	-2.466	1.00	23.08
1311	CB	LEU	A	368	28.576	18.913	-1.070	1.00	23.25
1312	CG	LEU	A	368	29.713	19.763	-0.491	1.00	23.11
1313	CD1	LEU	A	368	29.369	20.196	0.932	1.00	22.57

1314	CD2	LEU	A	368	31.002	18.960	-0.492	1.00	24.48
1315	C	LEU	A	368	27.681	17.382	-2.834	1.00	22.79
1316	O	LEU	A	368	27.542	16.306	-2.250	1.00	22.44
1317	N	GLU	A	369	26.862	17.796	-3.796	1.00	22.82
1318	CA	GLU	A	369	25.744	16.983	-4.260	1.00	24.48
1319	CB	GLU	A	369	26.279	15.731	-4.955	1.00	26.99
1320	CG	GLU	A	369	26.173	15.757	-6.461	1.00	33.00
1321	CD	GLU	A	369	26.960	14.633	-7.104	1.00	35.36
1322	OE1	GLU	A	369	26.965	13.513	-6.547	1.00	37.48
1323	OE2	GLU	A	369	27.568	14.870	-8.166	1.00	36.92
1324	C	GLU	A	369	24.778	16.571	-3.155	1.00	22.38
1325	O	GLU	A	369	24.286	15.445	-3.144	1.00	23.39
1326	N	LEU	A	370	24.507	17.476	-2.221	1.00	21.57
1327	CA	LEU	A	370	23.586	17.168	-1.133	1.00	18.06
1328	CB	LEU	A	370	23.717	18.197	-0.009	1.00	18.81
1329	CG	LEU	A	370	25.064	18.386	0.688	1.00	16.97
1330	CD1	LEU	A	370	24.875	19.342	1.856	1.00	16.61
1331	CD2	LEU	A	370	25.578	17.044	1.194	1.00	18.25
1332	C	LEU	A	370	22.148	17.199	-1.635	1.00	18.75
1333	O	LEU	A	370	21.845	17.849	-2.639	1.00	19.00
1334	N	ASP	A	371	21.272	16.476	-0.947	1.00	19.17
1335	CA	ASP	A	371	19.860	16.477	-1.292	1.00	18.60
1336	CB	ASP	A	371	19.336	15.060	-1.583	1.00	19.63
1337	CG	ASP	A	371	19.486	14.118	-0.411	1.00	21.42
1338	OD1	ASP	A	371	19.258	14.547	0.738	1.00	18.99
1339	OD2	ASP	A	371	19.813	12.934	-0.647	1.00	24.09
1340	C	ASP	A	371	19.152	17.091	-0.090	1.00	18.66
1341	O	ASP	A	371	19.789	17.388	0.919	1.00	19.31
1342	N	ASP	A	372	17.845	17.287	-0.190	1.00	18.35
1343	CA	ASP	A	372	17.098	17.902	0.896	1.00	18.08
1344	CB	ASP	A	372	15.641	18.084	0.477	1.00	20.09
1345	CG	ASP	A	372	15.487	19.092	-0.654	1.00	21.21
1346	OD1	ASP	A	372	15.925	20.253	-0.478	1.00	20.02

1347	OD2	ASP	A	372	14.932	18.728	-1.717	1.00	22.56
1348	C	ASP	A	372	17.189	17.174	2.236	1.00	17.57
1349	O	ASP	A	372	17.165	17.816	3.285	1.00	17.01
1350	N	SER	A	373	17.298	15.848	2.224	1.00	16.66
1351	CA	SER	A	373	17.406	15.132	3.493	1.00	17.74
1352	CB	SER	A	373	17.371	13.602	3.285	1.00	16.26
1353	OG	SER	A	373	18.514	13.111	2.609	1.00	18.96
1354	C	SER	A	373	18.697	15.552	4.201	1.00	17.27
1355	O	SER	A	373	18.723	15.696	5.423	1.00	19.27
1356	N	ASP	A	374	19.763	15.765	3.433	1.00	16.48
1357	CA	ASP	A	374	21.045	16.188	4.007	1.00	15.88
1358	CB	ASP	A	374	22.174	16.142	2.969	1.00	15.19
1359	CG	ASP	A	374	22.316	14.795	2.301	1.00	18.19
1360	OD1	ASP	A	374	22.362	13.768	3.014	1.00	19.73
1361	OD2	ASP	A	374	22.404	14.777	1.053	1.00	17.35
1362	C	ASP	A	374	20.947	17.631	4.494	1.00	15.34
1363	O	ASP	A	374	21.355	17.954	5.608	1.00	13.16
1364	N	ILE	A	375	20.418	18.492	3.629	1.00	14.16
1365	CA	ILE	A	375	20.283	19.912	3.924	1.00	14.77
1366	CB	ILE	A	375	19.667	20.661	2.713	1.00	14.32
1367	CG2	ILE	A	375	19.457	22.126	3.054	1.00	13.42
1368	CG1	ILE	A	375	20.598	20.528	1.506	1.00	12.81
1369	CD1	ILE	A	375	19.942	20.836	0.159	1.00	10.35
1370	C	ILE	A	375	19.456	20.185	5.178	1.00	15.58
1371	O	ILE	A	375	19.812	21.039	5.993	1.00	15.62
1372	N	SER	A	376	18.363	19.449	5.347	1.00	15.94
1373	CA	SER	A	376	17.517	19.656	6.516	1.00	17.39
1374	CB	SER	A	376	16.329	18.691	6.509	1.00	18.46
1375	OG	SER	A	376	16.754	17.354	6.681	1.00	19.88
1376	C	SER	A	376	18.313	19.472	7.799	1.00	16.76
1377	O	SER	A	376	18.141	20.231	8.740	1.00	15.46
1378	N	LEU	A	377	19.179	18.462	7.839	1.00	17.17
1379	CA	LEU	A	377	19.985	18.213	9.036	1.00	18.15

1380	CB	LEU	A	377	20.649	16.825	8.966	1.00	18.31
1381	CG	LEU	A	377	19.691	15.629	8.897	1.00	20.80
1382	CD1	LEU	A	377	20.471	14.320	8.902	1.00	22.15
1383	CD2	LEU	A	377	18.737	15.675	10.085	1.00	22.01
1384	C	LEU	A	377	21.058	19.285	9.203	1.00	17.32
1385	O	LEU	A	377	21.344	19.720	10.317	1.00	17.55
1386	N	PHE	A	378	21.650	19.697	8.085	1.00	15.68
1387	CA	PHE	A	378	22.694	20.723	8.085	1.00	15.42
1388	CB	PHE	A	378	23.185	20.951	6.652	1.00	14.83
1389	CG	PHE	A	378	24.352	21.895	6.547	1.00	17.91
1390	CD1	PHE	A	378	25.627	21.491	6.928	1.00	18.12
1391	CD2	PHE	A	378	24.172	23.191	6.070	1.00	17.17
1392	CE1	PHE	A	378	26.709	22.364	6.835	1.00	19.84
1393	CE2	PHE	A	378	25.248	24.072	5.974	1.00	17.27
1394	CZ	PHE	A	378	26.519	23.657	6.357	1.00	18.98
1395	C	PHE	A	378	22.138	22.032	8.664	1.00	14.65
1396	O	PHE	A	378	22.778	22.688	9.489	1.00	14.80
1397	N	VAL	A	379	20.937	22.403	8.230	1.00	14.52
1398	CA	VAL	A	379	20.305	23.625	8.713	1.00	13.14
1399	CB	VAL	A	379	19.060	23.964	7.861	1.00	14.31
1400	CG1	VAL	A	379	18.258	25.093	8.492	1.00	13.46
1401	CG2	VAL	A	379	19.520	24.388	6.460	1.00	13.68
1402	C	VAL	A	379	19.945	23.536	10.200	1.00	14.97
1403	O	VAL	A	379	20.093	24.511	10.942	1.00	14.16
1404	N	ALA	A	380	19.479	22.372	10.642	1.00	14.60
1405	CA	ALA	A	380	19.139	22.212	12.055	1.00	15.75
1406	CB	ALA	A	380	18.541	20.830	12.313	1.00	14.49
1407	C	ALA	A	380	20.412	22.389	12.875	1.00	17.48
1408	O	ALA	A	380	20.388	22.955	13.967	1.00	18.76
1409	N	ALA	A	381	21.521	21.890	12.337	1.00	17.47
1410	CA	ALA	A	381	22.809	21.989	13.008	1.00	18.52
1411	CB	ALA	A	381	23.843	21.138	12.275	1.00	18.08
1412	C	ALA	A	381	23.295	23.440	13.116	1.00	18.95

1413	O	ALA	A	381	23.826	23.843	14.149	1.00	18.98
1414	N	ILE	A	382	23.120	24.237	12.065	1.00	18.97
1415	CA	ILE	A	382	23.582	25.621	12.157	1.00	19.61
1416	CB	ILE	A	382	23.589	26.346	10.767	1.00	22.32
1417	CG2	ILE	A	382	24.054	25.408	9.685	1.00	22.00
1418	CG1	ILE	A	382	22.217	26.918	10.442	1.00	25.81
1419	CD1	ILE	A	382	21.988	28.285	11.051	1.00	26.92
1420	C	ILE	A	382	22.722	26.408	13.152	1.00	19.24
1421	O	ILE	A	382	23.223	27.278	13.869	1.00	18.21
1422	N	ILE	A	383	21.434	26.086	13.209	1.00	17.90
1423	CA	ILE	A	383	20.518	26.775	14.113	1.00	18.91
1424	CB	ILE	A	383	19.049	26.426	13.786	1.00	20.25
1425	CG2	ILE	A	383	18.122	26.923	14.899	1.00	20.50
1426	CG1	ILE	A	383	18.655	27.055	12.446	1.00	19.74
1427	CD1	ILE	A	383	17.224	26.779	12.032	1.00	20.27
1428	C	ILE	A	383	20.788	26.438	15.578	1.00	19.83
1429	O	ILE	A	383	20.882	27.328	16.426	1.00	18.98
1430	N	CYS	A	384	20.930	25.154	15.876	1.00	21.71
1431	CA	CYS	A	384	21.169	24.735	17.253	1.00	24.63
1432	CB	CYS	A	384	20.583	23.343	17.466	1.00	26.05
1433	SG	CYS	A	384	18.829	23.300	17.088	1.00	27.14
1434	C	CYS	A	384	22.653	24.763	17.576	1.00	25.29
1435	O	CYS	A	384	23.277	23.732	17.827	1.00	26.58
1436	N	CYS	A	385	23.197	25.974	17.564	1.00	27.00
1437	CA	CYS	A	385	24.605	26.233	17.822	1.00	28.30
1438	CB	CYS	A	385	25.104	27.255	16.804	1.00	30.14
1439	SG	CYS	A	385	26.815	27.715	16.976	1.00	32.84
1440	C	CYS	A	385	24.816	26.764	19.243	1.00	27.82
1441	O	CYS	A	385	24.267	27.801	19.615	1.00	27.12
1442	N	GLY	A	386	25.624	26.055	20.026	1.00	28.23
1443	CA	GLY	A	386	25.872	26.464	21.398	1.00	28.09
1444	C	GLY	A	386	26.927	27.539	21.582	1.00	28.17
1445	O	GLY	A	386	27.159	27.987	22.702	1.00	30.05

1446	N	ASP	A	387	27.555	27.965	20.490	1.00	29.00
1447	CA	ASP	A	387	28.602	28.982	20.555	1.00	29.78
1448	CB	ASP	A	387	29.691	28.690	19.520	1.00	33.93
1449	CG	ASP	A	387	30.174	27.263	19.569	1.00	37.57
1450	OD1	ASP	A	387	30.417	26.758	20.687	1.00	40.66
1451	OD2	ASP	A	387	30.320	26.651	18.489	1.00	39.44
1452	C	ASP	A	387	28.107	30.404	20.330	1.00	27.38
1453	O	ASP	A	387	28.889	31.348	20.396	1.00	27.02
1454	N	ARG	A	388	26.818	30.563	20.057	1.00	25.37
1455	CA	ARG	A	388	26.271	31.889	19.807	1.00	24.60
1456	CB	ARG	A	388	24.785	31.791	19.462	1.00	23.34
1457	CG	ARG	A	388	24.471	30.855	18.309	1.00	19.60
1458	CD	ARG	A	388	25.262	31.214	17.061	1.00	20.49
1459	NE	ARG	A	388	24.765	30.481	15.900	1.00	14.79
1460	CZ	ARG	A	388	25.332	30.498	14.700	1.00	16.61
1461	NH1	ARG	A	388	26.430	31.215	14.489	1.00	14.39
1462	NH2	ARG	A	388	24.798	29.789	13.714	1.00	14.57
1463	C	ARG	A	388	26.457	32.840	20.987	1.00	26.30
1464	O	ARG	A	388	26.286	32.458	22.143	1.00	26.77
1465	N	PRO	A	389	26.821	34.098	20.704	1.00	27.02
1466	CD	PRO	A	389	27.215	34.629	19.388	1.00	26.91
1467	CA	PRO	A	389	27.025	35.101	21.752	1.00	27.46
1468	CB	PRO	A	389	27.454	36.338	20.966	1.00	28.18
1469	CG	PRO	A	389	28.135	35.762	19.770	1.00	28.30
1470	C	PRO	A	389	25.739	35.352	22.539	1.00	28.08
1471	O	PRO	A	389	24.643	35.288	21.982	1.00	28.60
1472	N	GLY	A	390	25.881	35.620	23.834	1.00	27.99
1473	CA	GLY	A	390	24.731	35.912	24.674	1.00	27.31
1474	C	GLY	A	390	23.805	34.779	25.077	1.00	26.48
1475	O	GLY	A	390	22.720	35.038	25.601	1.00	25.44
1476	N	LEU	A	391	24.207	33.534	24.841	1.00	25.96
1477	CA	LEU	A	391	23.369	32.396	25.211	1.00	26.11
1478	CB	LEU	A	391	23.808	31.132	24.474	1.00	26.09

1479	CG	LEU	A	391	23.410	30.999	23.004	1.00	25.05
1480	CD1	LEU	A	391	24.037	29.734	22.431	1.00	23.61
1481	CD2	LEU	A	391	21.895	30.941	22.884	1.00	23.97
1482	C	LEU	A	391	23.430	32.135	26.708	1.00	27.86
1483	O	LEU	A	391	24.468	32.340	27.341	1.00	26.88
1484	N	LEU	A	392	22.318	31.662	27.260	1.00	28.14
1485	CA	LEU	A	392	22.230	31.366	28.682	1.00	31.00
1486	CB	LEU	A	392	20.863	31.794	29.225	1.00	30.68
1487	CG	LEU	A	392	20.575	31.444	30.690	1.00	32.59
1488	CD1	LEU	A	392	21.613	32.099	31.595	1.00	32.90
1489	CD2	LEU	A	392	19.173	31.906	31.057	1.00	31.69
1490	C	LEU	A	392	22.428	29.883	28.943	1.00	31.60
1491	O	LEU	A	392	23.371	29.471	29.618	1.00	33.05
1492	N	ASN	A	393	21.527	29.084	28.388	1.00	31.62
1493	CA	ASN	A	393	21.555	27.642	28.565	1.00	32.32
1494	CB	ASN	A	393	20.136	27.109	28.403	1.00	34.00
1495	CG	ASN	A	393	19.940	25.769	29.056	1.00	36.18
1496	OD1	ASN	A	393	18.821	25.265	29.121	1.00	38.80
1497	ND2	ASN	A	393	21.025	25.178	29.547	1.00	37.30
1498	C	ASN	A	393	22.501	26.938	27.586	1.00	31.82
1499	O	ASN	A	393	22.112	25.986	26.913	1.00	30.71
1500	N	VAL	A	394	23.743	27.406	27.526	1.00	31.16
1501	CA	VAL	A	394	24.748	26.838	26.634	1.00	31.48
1502	CB	VAL	A	394	26.140	27.467	26.912	1.00	31.26
1503	CG1	VAL	A	394	26.485	27.325	28.385	1.00	32.59
1504	CG2	VAL	A	394	27.204	26.802	26.049	1.00	31.72
1505	C	VAL	A	394	24.843	25.311	26.739	1.00	31.80
1506	O	VAL	A	394	24.984	24.619	25.728	1.00	32.39
1507	N	GLY	A	395	24.753	24.789	27.958	1.00	30.80
1508	CA	GLY	A	395	24.834	23.351	28.150	1.00	30.87
1509	C	GLY	A	395	23.747	22.558	27.443	1.00	31.11
1510	O	GLY	A	395	24.037	21.612	26.707	1.00	31.28
1511	N	HIS	A	396	22.493	22.940	27.662	1.00	30.39

1512	CA	HIS	A	396	21.370	22.248	27.047	1.00	30.64
1513	CB	HIS	A	396	20.046	22.779	27.613	1.00	33.97
1514	CG	HIS	A	396	19.864	22.503	29.077	1.00	38.64
1515	CD2	HIS	A	396	18.831	22.763	29.914	1.00	40.99
1516	ND1	HIS	A	396	20.841	21.913	29.849	1.00	39.58
1517	CE1	HIS	A	396	20.420	21.824	31.098	1.00	41.27
1518	NE2	HIS	A	396	19.204	22.334	31.165	1.00	41.61
1519	C	HIS	A	396	21.386	22.376	25.526	1.00	29.36
1520	O	HIS	A	396	20.970	21.465	24.821	1.00	28.36
1521	N	ILE	A	397	21.873	23.504	25.022	1.00	27.89
1522	CA	ILE	A	397	21.935	23.707	23.579	1.00	27.60
1523	CB	ILE	A	397	22.208	25.194	23.240	1.00	25.64
1524	CG2	ILE	A	397	22.465	25.366	21.743	1.00	25.46
1525	CG1	ILE	A	397	20.998	26.036	23.649	1.00	23.43
1526	CD1	ILE	A	397	21.234	27.535	23.573	1.00	23.81
1527	C	ILE	A	397	23.014	22.817	22.961	1.00	28.42
1528	O	ILE	A	397	22.837	22.292	21.863	1.00	28.52
1529	N	GLU	A	398	24.124	22.635	23.671	1.00	28.38
1530	CA	GLU	A	398	25.202	21.789	23.167	1.00	30.86
1531	CB	GLU	A	398	26.423	21.850	24.091	1.00	31.87
1532	CG	GLU	A	398	27.051	23.224	24.207	1.00	35.51
1533	CD	GLU	A	398	28.340	23.206	25.006	1.00	37.24
1534	OE1	GLU	A	398	28.347	22.630	26.114	1.00	38.47
1535	OE2	GLU	A	398	29.342	23.776	24.526	1.00	39.11
1536	C	GLU	A	398	24.743	20.339	23.037	1.00	30.96
1537	O	GLU	A	398	25.105	19.655	22.084	1.00	32.65
1538	N	LYS	A	399	23.950	19.870	23.996	1.00	31.74
1539	CA	LYS	A	399	23.457	18.495	23.966	1.00	32.12
1540	CB	LYS	A	399	22.721	18.166	25.272	1.00	34.57
1541	CG	LYS	A	399	21.269	18.617	25.317	1.00	37.40
1542	CD	LYS	A	399	20.332	17.512	24.854	1.00	39.89
1543	CE	LYS	A	399	19.038	18.078	24.284	1.00	40.38
1544	NZ	LYS	A	399	18.417	19.102	25.174	1.00	42.06

1545	C	LYS	A	399	22.522	18.335	22.770	1.00	30.88
1546	O	LYS	A	399	22.437	17.264	22.166	1.00	29.64
1547	N	MET	A	400	21.823	19.413	22.433	1.00	30.20
1548	CA	MET	A	400	20.909	19.408	21.298	1.00	30.04
1549	CB	MET	A	400	20.125	20.719	21.248	1.00	31.30
1550	CG	MET	A	400	18.626	20.562	21.377	1.00	34.42
1551	SD	MET	A	400	17.780	22.138	21.146	1.00	37.50
1552	CE	MET	A	400	17.589	22.649	22.799	1.00	35.32
1553	C	MET	A	400	21.705	19.251	20.006	1.00	28.14
1554	O	MET	A	400	21.406	18.386	19.177	1.00	27.06
1555	N	GLN	A	401	22.719	20.095	19.836	1.00	27.24
1556	CA	GLN	A	401	23.548	20.044	18.638	1.00	27.85
1557	CB	GLN	A	401	24.571	21.188	18.628	1.00	29.46
1558	CG	GLN	A	401	25.434	21.214	17.366	1.00	32.43
1559	CD	GLN	A	401	26.273	22.480	17.228	1.00	34.32
1560	OE1	GLN	A	401	27.074	22.809	18.102	1.00	34.44
1561	NE2	GLN	A	401	26.093	23.190	16.118	1.00	32.43
1562	C	GLN	A	401	24.269	18.705	18.539	1.00	27.48
1563	O	GLN	A	401	24.474	18.184	17.445	1.00	26.07
1564	N	GLU	A	402	24.641	18.149	19.687	1.00	27.34
1565	CA	GLU	A	402	25.334	16.865	19.729	1.00	28.25
1566	CB	GLU	A	402	25.617	16.464	21.184	1.00	30.37
1567	CG	GLU	A	402	26.263	15.089	21.339	1.00	35.80
1568	CD	GLU	A	402	26.573	14.744	22.787	1.00	38.57
1569	OE1	GLU	A	402	27.527	15.326	23.347	1.00	39.33
1570	OE2	GLU	A	402	25.856	13.895	23.365	1.00	39.79
1571	C	GLU	A	402	24.504	15.782	19.044	1.00	26.37
1572	O	GLU	A	402	25.017	15.030	18.216	1.00	26.12
1573	N	GLY	A	403	23.223	15.714	19.398	1.00	22.95
1574	CA	GLY	A	403	22.335	14.727	18.814	1.00	22.23
1575	C	GLY	A	403	22.119	14.941	17.326	1.00	22.14
1576	O	GLY	A	403	22.068	13.985	16.553	1.00	22.69
1577	N	ILE	A	404	21.991	16.199	16.918	1.00	20.27

1578	CA	ILE	A	404	21.790	16.528	15.508	1.00	20.28
1579	CB	ILE	A	404	21.501	18.047	15.333	1.00	18.92
1580	CG2	ILE	A	404	21.570	18.439	13.853	1.00	18.08
1581	CG1	ILE	A	404	20.130	18.370	15.931	1.00	20.64
1582	CD1	ILE	A	404	19.754	19.853	15.927	1.00	21.12
1583	C	ILE	A	404	23.012	16.129	14.683	1.00	20.45
1584	O	ILE	A	404	22.885	15.494	13.634	1.00	19.39
1585	N	VAL	A	405	24.195	16.491	15.170	1.00	22.04
1586	CA	VAL	A	405	25.441	16.167	14.484	1.00	24.01
1587	CB	VAL	A	405	26.654	16.764	15.229	1.00	24.63
1588	CG1	VAL	A	405	27.950	16.264	14.608	1.00	26.70
1589	CG2	VAL	A	405	26.597	18.282	15.168	1.00	25.08
1590	C	VAL	A	405	25.623	14.656	14.376	1.00	24.35
1591	O	VAL	A	405	26.062	14.145	13.347	1.00	24.50
1592	N	HIS	A	406	25.286	13.951	15.451	1.00	24.73
1593	CA	HIS	A	406	25.393	12.499	15.494	1.00	25.40
1594	CB	HIS	A	406	24.870	11.980	16.834	1.00	27.91
1595	CG	HIS	A	406	24.719	10.492	16.890	1.00	29.97
1596	CD2	HIS	A	406	23.623	9.704	16.779	1.00	31.72
1597	ND1	HIS	A	406	25.790	9.638	17.041	1.00	32.64
1598	CE1	HIS	A	406	25.362	8.388	17.020	1.00	31.24
1599	NE2	HIS	A	406	24.051	8.400	16.861	1.00	32.29
1600	C	HIS	A	406	24.573	11.891	14.362	1.00	24.78
1601	O	HIS	A	406	25.073	11.085	13.573	1.00	23.70
1602	N	VAL	A	407	23.306	12.287	14.297	1.00	24.16
1603	CA	VAL	A	407	22.394	11.797	13.276	1.00	24.60
1604	CB	VAL	A	407	20.962	12.319	13.536	1.00	26.47
1605	CG1	VAL	A	407	20.059	12.000	12.360	1.00	29.88
1606	CG2	VAL	A	407	20.412	11.675	14.805	1.00	27.86
1607	C	VAL	A	407	22.872	12.218	11.885	1.00	23.32
1608	O	VAL	A	407	22.752	11.455	10.922	1.00	21.28
1609	N	LEU	A	408	23.430	13.422	11.785	1.00	21.40
1610	CA	LEU	A	408	23.939	13.914	10.510	1.00	20.88

1611	CB	LEU	A	408	24.388	15.378	10.636	1.00	20.25
1612	CG	LEU	A	408	25.166	15.976	9.458	1.00	19.60
1613	CD1	LEU	A	408	24.324	15.912	8.188	1.00	18.77
1614	CD2	LEU	A	408	25.545	17.412	9.770	1.00	20.66
1615	C	LEU	A	408	25.108	13.058	10.026	1.00	21.76
1616	O	LEU	A	408	25.145	12.653	8.867	1.00	21.23
1617	N	ARG	A	409	26.057	12.776	10.917	1.00	22.31
1618	CA	ARG	A	409	27.217	11.971	10.547	1.00	23.13
1619	CB	ARG	A	409	28.170	11.788	11.736	1.00	25.75
1620	CG	ARG	A	409	29.480	11.102	11.332	1.00	30.84
1621	CD	ARG	A	409	30.361	10.722	12.517	1.00	34.64
1622	NE	ARG	A	409	30.566	11.828	13.444	1.00	36.72
1623	CZ	ARG	A	409	29.936	11.949	14.607	1.00	38.12
1624	NH1	ARG	A	409	29.063	11.027	14.986	1.00	40.03
1625	NH2	ARG	A	409	30.175	12.993	15.390	1.00	40.43
1626	C	ARG	A	409	26.800	10.598	10.039	1.00	23.39
1627	O	ARG	A	409	27.345	10.093	9.056	1.00	22.61
1628	N	LEU	A	410	25.835	9.991	10.718	1.00	22.60
1629	CA	LEU	A	410	25.351	8.673	10.332	1.00	24.37
1630	CB	LEU	A	410	24.452	8.106	11.438	1.00	24.59
1631	CG	LEU	A	410	25.217	7.686	12.701	1.00	27.68
1632	CD1	LEU	A	410	24.251	7.309	13.813	1.00	27.24
1633	CD2	LEU	A	410	26.133	6.519	12.366	1.00	26.90
1634	C	LEU	A	410	24.595	8.737	9.007	1.00	23.58
1635	O	LEU	A	410	24.750	7.870	8.143	1.00	22.71
1636	N	HIS	A	411	23.786	9.776	8.844	1.00	22.55
1637	CA	HIS	A	411	23.015	9.944	7.618	1.00	22.81
1638	CB	HIS	A	411	22.097	11.168	7.741	1.00	22.24
1639	CG	HIS	A	411	21.156	11.337	6.590	1.00	22.11
1640	CD2	HIS	A	411	19.946	10.782	6.342	1.00	23.05
1641	ND1	HIS	A	411	21.437	12.140	5.505	1.00	23.65
1642	CE1	HIS	A	411	20.441	12.074	4.639	1.00	20.84
1643	NE2	HIS	A	411	19.524	11.256	5.122	1.00	24.45

1644	C	HIS	A	411	23.933	10.092	6.406	1.00	22.74
1645	O	HIS	A	411	23.689	9.497	5.351	1.00	21.42
1646	N	LEU	A	412	24.990	10.886	6.555	1.00	20.60
1647	CA	LEU	A	412	25.931	11.093	5.460	1.00	22.09
1648	CB	LEU	A	412	26.972	12.151	5.838	1.00	21.12
1649	CG	LEU	A	412	26.441	13.576	6.011	1.00	20.72
1650	CD1	LEU	A	412	27.572	14.496	6.451	1.00	20.64
1651	CD2	LEU	A	412	25.828	14.060	4.693	1.00	21.54
1652	C	LEU	A	412	26.640	9.806	5.063	1.00	22.50
1653	O	LEU	A	412	26.921	9.587	3.886	1.00	22.76
1654	N	GLN	A	413	26.944	8.960	6.041	1.00	24.45
1655	CA	GLN	A	413	27.622	7.702	5.748	1.00	26.41
1656	CB	GLN	A	413	28.021	6.987	7.043	1.00	28.87
1657	CG	GLN	A	413	29.245	7.579	7.714	1.00	32.50
1658	CD	GLN	A	413	30.154	6.519	8.306	1.00	35.70
1659	OE1	GLN	A	413	29.809	5.862	9.286	1.00	36.19
1660	NE2	GLN	A	413	31.326	6.343	7.702	1.00	38.34
1661	C	GLN	A	413	26.765	6.775	4.889	1.00	26.96
1662	O	GLN	A	413	27.271	6.120	3.976	1.00	26.69
1663	N	SER	A	414	25.467	6.729	5.173	1.00	26.98
1664	CA	SER	A	414	24.555	5.877	4.417	1.00	27.71
1665	CB	SER	A	414	23.380	5.452	5.300	1.00	29.19
1666	OG	SER	A	414	22.560	6.558	5.632	1.00	33.45
1667	C	SER	A	414	24.017	6.521	3.138	1.00	26.94
1668	O	SER	A	414	23.709	5.820	2.175	1.00	27.54
1669	N	ASN	A	415	23.901	7.848	3.122	1.00	25.54
1670	CA	ASN	A	415	23.377	8.552	1.947	1.00	24.76
1671	CB	ASN	A	415	22.679	9.853	2.377	1.00	24.73
1672	CG	ASN	A	415	21.714	10.390	1.317	1.00	26.54
1673	OD1	ASN	A	415	21.324	11.562	1.350	1.00	25.37
1674	ND2	ASN	A	415	21.310	9.529	0.386	1.00	24.83
1675	C	ASN	A	415	24.472	8.870	0.927	1.00	24.23
1676	O	ASN	A	415	24.202	8.951	-0.271	1.00	23.51

1677	N	HIS	A	416	25.704	9.053	1.403	1.00	23.19
1678	CA	HIS	A	416	26.837	9.354	0.526	1.00	24.23
1679	CB	HIS	A	416	27.273	10.820	0.674	1.00	22.51
1680	CG	HIS	A	416	26.236	11.811	0.239	1.00	21.91
1681	CD2	HIS	A	416	25.999	12.381	-0.967	1.00	19.28
1682	ND1	HIS	A	416	25.279	12.314	1.094	1.00	22.80
1683	CE1	HIS	A	416	24.497	13.152	0.434	1.00	17.33
1684	NE2	HIS	A	416	24.912	13.210	-0.819	1.00	20.76
1685	C	HIS	A	416	28.019	8.445	0.859	1.00	26.11
1686	O	HIS	A	416	29.076	8.912	1.285	1.00	24.94
1687	N	PRO	A	417	27.859	7.131	0.647	1.00	29.11
1688	CD	PRO	A	417	26.708	6.470	0.007	1.00	29.49
1689	CA	PRO	A	417	28.920	6.163	0.935	1.00	30.85
1690	CB	PRO	A	417	28.241	4.824	0.656	1.00	31.26
1691	CG	PRO	A	417	27.314	5.162	-0.472	1.00	30.77
1692	C	PRO	A	417	30.193	6.350	0.118	1.00	33.62
1693	O	PRO	A	417	31.264	5.895	0.524	1.00	35.12
1694	N	ASP	A	418	30.084	7.019	-1.025	1.00	34.60
1695	CA	ASP	A	418	31.247	7.230	-1.874	1.00	36.67
1696	CB	ASP	A	418	30.832	7.265	-3.349	1.00	39.63
1697	CG	ASP	A	418	30.147	5.981	-3.794	1.00	41.06
1698	OD1	ASP	A	418	30.576	4.893	-3.352	1.00	42.57
1699	OD2	ASP	A	418	29.188	6.058	-4.592	1.00	43.11
1700	C	ASP	A	418	32.048	8.483	-1.541	1.00	37.42
1701	O	ASP	A	418	33.252	8.534	-1.802	1.00	37.62
1702	N	ASP	A	419	31.399	9.492	-0.966	1.00	37.02
1703	CA	ASP	A	419	32.118	10.715	-0.632	1.00	37.69
1704	CB	ASP	A	419	31.185	11.909	-0.446	1.00	36.87
1705	CG	ASP	A	419	31.953	13.225	-0.346	1.00	37.47
1706	OD1	ASP	A	419	33.059	13.232	0.238	1.00	36.42
1707	OD2	ASP	A	419	31.455	14.253	-0.845	1.00	37.98
1708	C	ASP	A	419	32.953	10.566	0.620	1.00	38.20
1709	O	ASP	A	419	32.444	10.440	1.736	1.00	37.99

1710	N	ILE	A	420	34.255	10.612	0.399	1.00	39.15
1711	CA	ILE	A	420	35.263	10.494	1.429	1.00	37.95
1712	CB	ILE	A	420	36.621	10.896	0.829	1.00	39.91
1713	CG2	ILE	A	420	37.041	9.869	-0.219	1.00	40.60
1714	CG1	ILE	A	420	36.499	12.270	0.150	1.00	41.10
1715	CD1	ILE	A	420	37.772	12.762	-0.510	1.00	42.96
1716	C	ILE	A	420	35.022	11.292	2.716	1.00	35.07
1717	O	ILE	A	420	34.524	10.764	3.711	1.00	35.43
1718	N	PHE	A	421	35.380	12.568	2.685	1.00	31.63
1719	CA	PHE	A	421	35.264	13.435	3.846	1.00	26.48
1720	CB	PHE	A	421	36.496	14.341	3.943	1.00	29.04
1721	CG	PHE	A	421	37.809	13.614	3.925	1.00	30.93
1722	CD1	PHE	A	421	38.353	13.160	2.733	1.00	33.42
1723	CD2	PHE	A	421	38.524	13.423	5.100	1.00	31.75
1724	CE1	PHE	A	421	39.599	12.529	2.709	1.00	34.29
1725	CE2	PHE	A	421	39.768	12.794	5.089	1.00	31.88
1726	CZ	PHE	A	421	40.306	12.348	3.892	1.00	33.09
1727	C	PHE	A	421	34.039	14.339	3.827	1.00	23.47
1728	O	PHE	A	421	34.156	15.505	4.176	1.00	21.09
1729	N	LEU	A	422	32.869	13.832	3.449	1.00	20.27
1730	CA	LEU	A	422	31.704	14.715	3.403	1.00	17.44
1731	CB	LEU	A	422	30.476	13.972	2.851	1.00	15.99
1732	CG	LEU	A	422	29.237	14.847	2.598	1.00	14.82
1733	CD1	LEU	A	422	29.607	16.092	1.808	1.00	15.78
1734	CD2	LEU	A	422	28.190	14.039	1.867	1.00	16.91
1735	C	LEU	A	422	31.376	15.381	4.745	1.00	17.17
1736	O	LEU	A	422	30.989	16.561	4.784	1.00	15.16
1737	N	PHE	A	423	31.537	14.656	5.850	1.00	15.85
1738	CA	PHE	A	423	31.242	15.247	7.154	1.00	15.61
1739	CB	PHE	A	423	31.333	14.189	8.264	1.00	17.14
1740	CG	PHE	A	423	30.974	14.708	9.626	1.00	18.64
1741	CD1	PHE	A	423	29.698	15.202	9.888	1.00	20.33
1742	CD2	PHE	A	423	31.910	14.705	10.651	1.00	20.31

1743	CE1	PHE	A	423	29.360	15.685	11.157	1.00	20.29
1744	CE2	PHE	A	423	31.583	15.186	11.924	1.00	21.44
1745	CZ	PHE	A	423	30.305	15.676	12.175	1.00	22.31
1746	C	PHE	A	423	32.194	16.416	7.451	1.00	16.28
1747	O	PHE	A	423	31.750	17.537	7.727	1.00	14.24
1748	N	PRO	A	424	33.519	16.174	7.416	1.00	17.45
1749	CD	PRO	A	424	34.280	14.915	7.331	1.00	17.91
1750	CA	PRO	A	424	34.397	17.313	7.697	1.00	16.84
1751	CB	PRO	A	424	35.797	16.680	7.749	1.00	19.13
1752	CG	PRO	A	424	35.657	15.406	6.971	1.00	18.96
1753	C	PRO	A	424	34.255	18.437	6.657	1.00	15.92
1754	O	PRO	A	424	34.467	19.610	6.966	1.00	15.44
1755	N	LYS	A	425	33.882	18.086	5.428	1.00	16.05
1756	CA	LYS	A	425	33.680	19.100	4.396	1.00	15.22
1757	CB	LYS	A	425	33.268	18.456	3.068	1.00	15.46
1758	CG	LYS	A	425	34.373	17.716	2.332	1.00	16.19
1759	CD	LYS	A	425	33.824	17.126	1.044	1.00	17.44
1760	CE	LYS	A	425	34.866	16.327	0.278	1.00	19.89
1761	NZ	LYS	A	425	34.278	15.771	-0.982	1.00	18.37
1762	C	LYS	A	425	32.561	20.034	4.850	1.00	14.66
1763	O	LYS	A	425	32.654	21.259	4.712	1.00	13.26
1764	N	LEU	A	426	31.497	19.445	5.394	1.00	13.97
1765	CA	LEU	A	426	30.351	20.219	5.864	1.00	14.01
1766	CB	LEU	A	426	29.155	19.301	6.136	1.00	14.60
1767	CG	LEU	A	426	28.490	18.720	4.887	1.00	18.11
1768	CD1	LEU	A	426	27.366	17.777	5.289	1.00	19.14
1769	CD2	LEU	A	426	27.948	19.859	4.027	1.00	19.11
1770	C	LEU	A	426	30.694	21.025	7.110	1.00	15.51
1771	O	LEU	A	426	30.200	22.138	7.290	1.00	16.69
1772	N	LEU	A	427	31.546	20.477	7.971	1.00	16.13
1773	CA	LEU	A	427	31.948	21.221	9.159	1.00	17.20
1774	CB	LEU	A	427	32.875	20.386	10.048	1.00	19.20
1775	CG	LEU	A	427	32.221	19.176	10.725	1.00	21.00

1776	CD1	LEU	A	427	33.248	18.435	11.574	1.00	22.86
1777	CD2	LEU	A	427	31.055	19.637	11.584	1.00	22.35
1778	C	LEU	A	427	32.669	22.480	8.691	1.00	17.44
1779	O	LEU	A	427	32.495	23.556	9.266	1.00	15.95
1780	N	GLN	A	428	33.480	22.357	7.643	1.00	16.16
1781	CA	GLN	A	428	34.183	23.532	7.134	1.00	16.84
1782	CB	GLN	A	428	35.235	23.150	6.087	1.00	17.05
1783	CG	GLN	A	428	36.001	24.372	5.560	1.00	20.71
1784	CD	GLN	A	428	36.981	24.039	4.453	1.00	22.77
1785	OE1	GLN	A	428	36.625	23.398	3.468	1.00	25.06
1786	NE2	GLN	A	428	38.224	24.488	4.606	1.00	26.03
1787	C	GLN	A	428	33.179	24.512	6.525	1.00	17.18
1788	O	GLN	A	428	33.333	25.728	6.656	1.00	17.33
1789	N	LYS	A	429	32.147	23.995	5.859	1.00	17.54
1790	CA	LYS	A	429	31.132	24.871	5.261	1.00	17.07
1791	CB	LYS	A	429	30.077	24.061	4.505	1.00	17.70
1792	CG	LYS	A	429	30.611	23.303	3.312	1.00	19.51
1793	CD	LYS	A	429	31.331	24.217	2.336	1.00	22.06
1794	CE	LYS	A	429	31.888	23.424	1.151	1.00	22.64
1795	NZ	LYS	A	429	32.800	24.262	0.326	1.00	21.64
1796	C	LYS	A	429	30.441	25.712	6.327	1.00	18.54
1797	O	LYS	A	429	30.070	26.865	6.079	1.00	16.97
1798	N	MET	A	430	30.258	25.136	7.513	1.00	18.74
1799	CA	MET	A	430	29.621	25.868	8.599	1.00	19.35
1800	CB	MET	A	430	29.418	24.957	9.810	1.00	22.86
1801	CG	MET	A	430	28.556	23.742	9.505	1.00	25.60
1802	SD	MET	A	430	28.185	22.755	10.953	1.00	29.86
1803	CE	MET	A	430	26.648	23.513	11.472	1.00	30.44
1804	C	MET	A	430	30.509	27.050	8.977	1.00	19.48
1805	O	MET	A	430	30.017	28.142	9.238	1.00	17.93
1806	N	ALA	A	431	31.819	26.824	9.010	1.00	19.56
1807	CA	ALA	A	431	32.768	27.883	9.345	1.00	18.57
1808	CB	ALA	A	431	34.160	27.293	9.551	1.00	20.87

1809	C	ALA	A	431	32.800	28.931	8.236	1.00	19.19
1810	O	ALA	A	431	32.910	30.136	8.498	1.00	18.72
1811	N	ASP	A	432	32.711	28.471	6.992	1.00	17.33
1812	CA	ASP	A	432	32.719	29.382	5.854	1.00	17.47
1813	CB	ASP	A	432	32.751	28.608	4.537	1.00	18.81
1814	CG	ASP	A	432	34.086	27.928	4.285	1.00	22.11
1815	OD1	ASP	A	432	35.085	28.306	4.925	1.00	23.74
1816	OD2	ASP	A	432	34.136	27.026	3.426	1.00	23.76
1817	C	ASP	A	432	31.477	30.268	5.890	1.00	17.16
1818	O	ASP	A	432	31.542	31.454	5.563	1.00	16.05
1819	N	LEU	A	433	30.349	29.691	6.296	1.00	15.92
1820	CA	LEU	A	433	29.097	30.442	6.367	1.00	15.51
1821	CB	LEU	A	433	27.919	29.500	6.645	1.00	14.97
1822	CG	LEU	A	433	27.457	28.645	5.461	1.00	16.25
1823	CD1	LEU	A	433	26.435	27.633	5.928	1.00	15.43
1824	CD2	LEU	A	433	26.852	29.532	4.379	1.00	16.30
1825	C	LEU	A	433	29.148	31.523	7.436	1.00	16.51
1826	O	LEU	A	433	28.643	32.623	7.240	1.00	15.91
1827	N	ARG	A	434	29.756	31.207	8.573	1.00	17.51
1828	CA	ARG	A	434	29.857	32.181	9.651	1.00	19.49
1829	CB	ARG	A	434	30.546	31.554	10.863	1.00	20.19
1830	CG	ARG	A	434	30.526	32.444	12.094	1.00	24.32
1831	CD	ARG	A	434	30.936	31.678	13.331	1.00	27.77
1832	NE	ARG	A	434	29.962	30.650	13.689	1.00	30.42
1833	CZ	ARG	A	434	30.013	29.949	14.816	1.00	32.49
1834	NH1	ARG	A	434	30.992	30.171	15.682	1.00	33.93
1835	NH2	ARG	A	434	29.086	29.037	15.086	1.00	32.62
1836	C	ARG	A	434	30.644	33.397	9.162	1.00	19.24
1837	O	ARG	A	434	30.275	34.539	9.432	1.00	20.11
1838	N	GLN	A	435	31.730	33.145	8.441	1.00	20.35
1839	CA	GLN	A	435	32.554	34.224	7.905	1.00	21.41
1840	CB	GLN	A	435	33.828	33.656	7.272	1.00	23.62
1841	CG	GLN	A	435	34.616	34.659	6.435	1.00	28.57

1842	CD	GLN	A	435	35.501	35.574	7.260	1.00	33.29
1843	OE1	GLN	A	435	35.091	36.091	8.301	1.00	36.07
1844	NE2	GLN	A	435	36.725	35.789	6.788	1.00	36.08
1845	C	GLN	A	435	31.757	34.987	6.852	1.00	20.82
1846	O	GLN	A	435	31.773	36.217	6.814	1.00	19.43
1847	N	LEU	A	436	31.058	34.244	5.999	1.00	19.72
1848	CA	LEU	A	436	30.251	34.842	4.945	1.00	18.86
1849	CB	LEU	A	436	29.571	33.742	4.121	1.00	18.95
1850	CG	LEU	A	436	28.865	34.160	2.829	1.00	20.08
1851	CD1	LEU	A	436	29.911	34.595	1.800	1.00	20.86
1852	CD2	LEU	A	436	28.053	32.982	2.281	1.00	21.90
1853	C	LEU	A	436	29.187	35.783	5.525	1.00	18.74
1854	O	LEU	A	436	28.905	36.838	4.951	1.00	17.29
1855	N	VAL	A	437	28.592	35.401	6.655	1.00	17.24
1856	CA	VAL	A	437	27.561	36.235	7.283	1.00	17.47
1857	CB	VAL	A	437	26.774	35.456	8.361	1.00	17.76
1858	CG1	VAL	A	437	25.846	36.405	9.120	1.00	18.67
1859	CG2	VAL	A	437	25.945	34.348	7.700	1.00	14.52
1860	C	VAL	A	437	28.170	37.478	7.928	1.00	18.46
1861	O	VAL	A	437	27.615	38.576	7.834	1.00	18.68
1862	N	THR	A	438	29.309	37.301	8.588	1.00	18.45
1863	CA	THR	A	438	29.984	38.418	9.237	1.00	19.82
1864	CB	THR	A	438	31.316	37.969	9.877	1.00	20.76
1865	OG1	THR	A	438	31.058	36.955	10.856	1.00	22.73
1866	CG2	THR	A	438	32.006	39.146	10.551	1.00	23.28
1867	C	THR	A	438	30.271	39.498	8.204	1.00	20.08
1868	O	THR	A	438	30.034	40.685	8.440	1.00	20.49
1869	N	GLU	A	439	30.778	39.071	7.052	1.00	18.53
1870	CA	GLU	A	439	31.104	39.983	5.972	1.00	19.18
1871	CB	GLU	A	439	31.900	39.236	4.897	1.00	19.51
1872	CG	GLU	A	439	33.061	38.440	5.491	1.00	23.78
1873	CD	GLU	A	439	33.912	37.735	4.455	1.00	25.56
1874	OE1	GLU	A	439	33.347	37.165	3.502	1.00	27.66

1875	OE2	GLU	A	439	35.152	37.738	4.607	1.00	27.05
1876	C	GLU	A	439	29.852	40.617	5.369	1.00	17.55
1877	O	GLU	A	439	29.862	41.786	4.988	1.00	18.18
1878	N	HIS	A	440	28.774	39.843	5.279	1.00	16.47
1879	CA	HIS	A	440	27.527	40.353	4.725	1.00	15.35
1880	CB	HIS	A	440	26.512	39.217	4.561	1.00	13.45
1881	CG	HIS	A	440	25.169	39.663	4.063	1.00	13.44
1882	CD2	HIS	A	440	24.005	39.879	4.719	1.00	14.46
1883	ND1	HIS	A	440	24.913	39.927	2.734	1.00	14.54
1884	CE1	HIS	A	440	23.649	40.284	2.593	1.00	14.39
1885	NE2	HIS	A	440	23.076	40.265	3.783	1.00	14.22
1886	C	HIS	A	440	26.947	41.444	5.627	1.00	15.34
1887	O	HIS	A	440	26.494	42.474	5.139	1.00	16.88
1888	N	ALA	A	441	26.956	41.216	6.936	1.00	16.12
1889	CA	ALA	A	441	26.425	42.197	7.879	1.00	17.96
1890	CB	ALA	A	441	26.513	41.661	9.305	1.00	17.75
1891	C	ALA	A	441	27.190	43.518	7.773	1.00	19.46
1892	O	ALA	A	441	26.619	44.594	7.956	1.00	18.94
1893	N	GLN	A	442	28.483	43.431	7.479	1.00	21.32
1894	CA	GLN	A	442	29.309	44.630	7.348	1.00	22.42
1895	CB	GLN	A	442	30.781	44.255	7.158	1.00	26.37
1896	CG	GLN	A	442	31.717	45.455	7.074	1.00	31.72
1897	CD	GLN	A	442	33.178	45.053	6.974	1.00	34.48
1898	OE1	GLN	A	442	33.675	44.272	7.786	1.00	37.93
1899	NE2	GLN	A	442	33.874	45.588	5.979	1.00	35.81
1900	C	GLN	A	442	28.831	45.449	6.157	1.00	21.76
1901	O	GLN	A	442	28.707	46.670	6.240	1.00	20.34
1902	N	LEU	A	443	28.557	44.771	5.047	1.00	19.43
1903	CA	LEU	A	443	28.087	45.452	3.851	1.00	20.58
1904	CB	LEU	A	443	28.060	44.491	2.661	1.00	21.26
1905	CG	LEU	A	443	27.571	45.092	1.339	1.00	23.72
1906	CD1	LEU	A	443	28.492	46.244	0.924	1.00	23.27
1907	CD2	LEU	A	443	27.542	44.016	0.268	1.00	23.43

1908	C	LEU	A	443	26.690	46.012	4.100	1.00	19.34
1909	O	LEU	A	443	26.373	47.114	3.663	1.00	20.88
1910	N	VAL	A	444	25.859	45.250	4.808	1.00	19.86
1911	CA	VAL	A	444	24.504	45.693	5.119	1.00	19.89
1912	CB	VAL	A	444	23.723	44.615	5.918	1.00	21.23
1913	CG1	VAL	A	444	22.357	45.155	6.342	1.00	22.52
1914	CG2	VAL	A	444	23.536	43.370	5.058	1.00	20.41
1915	C	VAL	A	444	24.557	46.992	5.928	1.00	21.15
1916	O	VAL	A	444	23.755	47.897	5.710	1.00	20.95
1917	N	GLN	A	445	25.512	47.083	6.849	1.00	21.46
1918	CA	GLN	A	445	25.663	48.278	7.672	1.00	23.89
1919	CB	GLN	A	445	26.722	48.047	8.752	1.00	27.62
1920	CG	GLN	A	445	26.863	49.191	9.753	1.00	32.28
1921	CD	GLN	A	445	25.636	49.366	10.638	1.00	35.43
1922	OE1	GLN	A	445	25.623	50.212	11.533	1.00	38.17
1923	NE2	GLN	A	445	24.602	48.567	10.395	1.00	37.92
1924	C	GLN	A	445	26.059	49.469	6.797	1.00	24.56
1925	O	GLN	A	445	25.586	50.588	7.003	1.00	22.97
1926	N	ILE	A	446	26.931	49.222	5.823	1.00	23.13
1927	CA	ILE	A	446	27.378	50.271	4.915	1.00	24.75
1928	CB	ILE	A	446	28.475	49.747	3.958	1.00	24.82
1929	CG2	ILE	A	446	28.747	50.759	2.855	1.00	24.01
1930	CG1	ILE	A	446	29.753	49.461	4.753	1.00	25.40
1931	CD1	ILE	A	446	30.852	48.807	3.946	1.00	25.53
1932	C	ILE	A	446	26.194	50.780	4.099	1.00	25.90
1933	O	ILE	A	446	25.990	51.989	3.968	1.00	26.44
1934	N	ILE	A	447	25.413	49.850	3.552	1.00	26.77
1935	CA	ILE	A	447	24.236	50.201	2.766	1.00	29.88
1936	CB	ILE	A	447	23.539	48.937	2.213	1.00	30.75
1937	CG2	ILE	A	447	22.150	49.299	1.663	1.00	33.39
1938	CG1	ILE	A	447	24.407	48.307	1.121	1.00	31.69
1939	CD1	ILE	A	447	23.811	47.036	0.510	1.00	34.09
1940	C	ILE	A	447	23.248	50.979	3.634	1.00	30.49

1941	O	ILE	A	447	22.670	51.979	3.206	1.00	30.43
1942	N	LYS	A	448	23.095	50.538	4.873	1.00	32.72
1943	CA	LYS	A	448	22.175	51.166	5.807	1.00	36.04
1944	CB	LYS	A	448	22.169	50.377	7.121	1.00	37.66
1945	CG	LYS	A	448	21.205	50.919	8.162	1.00	40.69
1946	CD	LYS	A	448	20.930	49.888	9.229	1.00	41.72
1947	CE	LYS	A	448	19.933	50.405	10.241	1.00	44.25
1948	NZ	LYS	A	448	20.486	51.487	11.103	1.00	45.65
1949	C	LYS	A	448	22.480	52.634	6.093	1.00	36.68
1950	O	LYS	A	448	21.566	53.450	6.206	1.00	36.26
1951	N	LYS	A	449	23.759	52.977	6.203	1.00	37.99
1952	CA	LYS	A	449	24.129	54.358	6.495	1.00	39.24
1953	CB	LYS	A	449	25.330	54.395	7.450	1.00	41.14
1954	CG	LYS	A	449	26.685	54.357	6.757	1.00	43.28
1955	CD	LYS	A	449	27.829	54.400	7.765	1.00	44.36
1956	CE	LYS	A	449	27.939	53.086	8.518	1.00	45.26
1957	NZ	LYS	A	449	28.212	51.958	7.586	1.00	44.67
1958	C	LYS	A	449	24.449	55.179	5.246	1.00	39.55
1959	O	LYS	A	449	24.523	56.408	5.307	1.00	39.79
1960	N	THR	A	450	24.630	54.502	4.117	1.00	39.02
1961	CA	THR	A	450	24.962	55.175	2.865	1.00	39.78
1962	CB	THR	A	450	26.150	54.462	2.168	1.00	40.83
1963	OG1	THR	A	450	27.381	54.930	2.736	1.00	41.96
1964	CG2	THR	A	450	26.149	54.722	0.671	1.00	42.44
1965	C	THR	A	450	23.802	55.298	1.879	1.00	39.33
1966	O	THR	A	450	23.724	56.263	1.120	1.00	39.15
1967	N	GLU	A	451	22.903	54.323	1.888	1.00	38.93
1968	CA	GLU	A	451	21.765	54.341	0.979	1.00	39.36
1969	CB	GLU	A	451	21.601	52.971	0.309	1.00	37.13
1970	CG	GLU	A	451	22.786	52.508	-0.542	1.00	33.20
1971	CD	GLU	A	451	22.987	53.336	-1.801	1.00	31.38
1972	OE1	GLU	A	451	21.993	53.869	-2.338	1.00	31.23
1973	OE2	GLU	A	451	24.140	53.436	-2.269	1.00	27.05

1974	C	GLU	A	451	20.480	54.701	1.718	1.00	41.61
1975	O	GLU	A	451	19.787	53.825	2.235	1.00	41.95
1976	N	SER	A	452	20.166	55.991	1.771	1.00	44.12
1977	CA	SER	A	452	18.955	56.445	2.444	1.00	46.91
1978	CB	SER	A	452	19.066	57.928	2.804	1.00	47.79
1979	OG	SER	A	452	20.074	58.140	3.781	1.00	49.02
1980	C	SER	A	452	17.767	56.216	1.521	1.00	48.12
1981	O	SER	A	452	16.611	56.306	1.933	1.00	48.49
1982	N	ASP	A	453	18.077	55.920	0.264	1.00	49.25
1983	CA	ASP	A	453	17.068	55.654	-0.750	1.00	50.01
1984	CB	ASP	A	453	17.754	55.278	-2.063	1.00	51.19
1985	CG	ASP	A	453	19.029	54.482	-1.845	1.00	51.21
1986	OD1	ASP	A	453	19.964	55.027	-1.223	1.00	52.21
1987	OD2	ASP	A	453	19.100	53.317	-2.288	1.00	52.20
1988	C	ASP	A	453	16.174	54.516	-0.287	1.00	49.54
1989	O	ASP	A	453	14.965	54.524	-0.513	1.00	50.36
1990	N	ALA	A	454	16.786	53.537	0.367	1.00	49.32
1991	CA	ALA	A	454	16.069	52.382	0.877	1.00	47.69
1992	CB	ALA	A	454	16.179	51.241	-0.102	1.00	48.66
1993	C	ALA	A	454	16.668	51.988	2.222	1.00	46.49
1994	O	ALA	A	454	17.885	51.940	2.373	1.00	47.87
1995	N	ALA	A	455	15.807	51.707	3.195	1.00	43.89
1996	CA	ALA	A	455	16.250	51.340	4.533	1.00	41.22
1997	CB	ALA	A	455	15.306	51.944	5.568	1.00	41.01
1998	C	ALA	A	455	16.341	49.829	4.724	1.00	39.82
1999	O	ALA	A	455	17.060	49.146	3.990	1.00	41.52
2000	N	LEU	A	456	15.625	49.329	5.728	1.00	36.01
2001	CA	LEU	A	456	15.580	47.904	6.063	1.00	32.30
2002	CB	LEU	A	456	16.744	47.508	6.981	1.00	33.09
2003	CG	LEU	A	456	18.083	47.052	6.390	1.00	33.05
2004	CD1	LEU	A	456	18.977	46.576	7.525	1.00	32.55
2005	CD2	LEU	A	456	17.870	45.925	5.391	1.00	31.55
2006	C	LEU	A	456	14.272	47.560	6.769	1.00	29.76

2007	O	LEU	A	456	13.758	48.345	7.574	1.00	26.72
2008	N	HIS	A	457	13.745	46.378	6.465	1.00	26.87
2009	CA	HIS	A	457	12.505	45.897	7.061	1.00	25.80
2010	CB	HIS	A	457	12.113	44.558	6.421	1.00	24.73
2011	CG	HIS	A	457	10.846	43.968	6.963	1.00	25.28
2012	CD2	HIS	A	457	10.567	43.401	8.160	1.00	24.58
2013	ND1	HIS	A	457	9.680	43.901	6.229	1.00	26.52
2014	CE1	HIS	A	457	8.740	43.316	6.950	1.00	25.66
2015	NE2	HIS	A	457	9.253	43.003	8.127	1.00	26.42
2016	C	HIS	A	457	12.711	45.716	8.567	1.00	25.90
2017	O	HIS	A	457	13.794	45.331	9.012	1.00	25.20
2018	N	PRO	A	458	11.669	45.995	9.368	1.00	25.60
2019	CD	PRO	A	458	10.368	46.543	8.941	1.00	26.08
2020	CA	PRO	A	458	11.719	45.868	10.829	1.00	25.42
2021	CB	PRO	A	458	10.257	46.032	11.229	1.00	25.91
2022	CG	PRO	A	458	9.777	47.043	10.243	1.00	27.38
2023	C	PRO	A	458	12.314	44.557	11.342	1.00	25.07
2024	O	PRO	A	458	13.151	44.559	12.246	1.00	25.29
2025	N	LEU	A	459	11.878	43.436	10.775	1.00	23.71
2026	CA	LEU	A	459	12.383	42.141	11.214	1.00	22.76
2027	CB	LEU	A	459	11.618	41.002	10.530	1.00	22.31
2028	CG	LEU	A	459	12.098	39.582	10.868	1.00	22.34
2029	CD1	LEU	A	459	11.955	39.318	12.368	1.00	23.76
2030	CD2	LEU	A	459	11.284	38.567	10.076	1.00	22.76
2031	C	LEU	A	459	13.872	41.998	10.930	1.00	22.18
2032	O	LEU	A	459	14.623	41.493	11.761	1.00	21.97
2033	N	LEU	A	460	14.301	42.438	9.753	1.00	21.66
2034	CA	LEU	A	460	15.710	42.337	9.397	1.00	21.60
2035	CB	LEU	A	460	15.892	42.619	7.902	1.00	20.70
2036	CG	LEU	A	460	14.974	41.760	7.022	1.00	19.18
2037	CD1	LEU	A	460	15.343	41.949	5.560	1.00	20.00
2038	CD2	LEU	A	460	15.098	40.285	7.418	1.00	16.85
2039	C	LEU	A	460	16.539	43.305	10.232	1.00	23.25

2040	O	LEU	A	460	17.679	43.015	10.606	1.00	21.71
2041	N	GLN	A	461	15.952	44.453	10.541	1.00	23.59
2042	CA	GLN	A	461	16.645	45.444	11.339	1.00	26.43
2043	CB	GLN	A	461	15.808	46.720	11.444	1.00	28.61
2044	CG	GLN	A	461	16.491	47.837	12.219	1.00	34.25
2045	CD	GLN	A	461	17.776	48.316	11.564	1.00	36.90
2046	OE1	GLN	A	461	18.513	49.110	12.145	1.00	40.50
2047	NE2	GLN	A	461	18.045	47.843	10.353	1.00	38.17
2048	C	GLN	A	461	16.950	44.899	12.734	1.00	25.75
2049	O	GLN	A	461	18.057	45.078	13.235	1.00	27.57
2050	N	GLU	A	462	15.989	44.224	13.361	1.00	25.39
2051	CA	GLU	A	462	16.241	43.696	14.699	1.00	26.81
2052	CB	GLU	A	462	14.930	43.290	15.401	1.00	28.93
2053	CG	GLU	A	462	14.134	42.155	14.784	1.00	30.21
2054	CD	GLU	A	462	12.838	41.880	15.553	1.00	32.16
2055	OE1	GLU	A	462	11.991	42.795	15.644	1.00	32.22
2056	OE2	GLU	A	462	12.665	40.755	16.071	1.00	30.73
2057	C	GLU	A	462	17.240	42.541	14.688	1.00	25.84
2058	O	GLU	A	462	17.970	42.332	15.659	1.00	25.91
2059	N	ILE	A	463	17.291	41.797	13.589	1.00	23.23
2060	CA	ILE	A	463	18.239	40.699	13.497	1.00	22.62
2061	CB	ILE	A	463	17.942	39.793	12.273	1.00	23.65
2062	CG2	ILE	A	463	19.115	38.833	12.020	1.00	21.96
2063	CG1	ILE	A	463	16.650	39.007	12.522	1.00	22.25
2064	CD1	ILE	A	463	16.196	38.160	11.338	1.00	24.20
2065	C	ILE	A	463	19.658	41.263	13.396	1.00	23.04
2066	O	ILE	A	463	20.568	40.782	14.062	1.00	20.73
2067	N	TYR	A	464	19.839	42.298	12.579	1.00	23.82
2068	CA	TYR	A	464	21.160	42.899	12.400	1.00	25.85
2069	CB	TYR	A	464	21.226	43.636	11.063	1.00	24.50
2070	CG	TYR	A	464	21.403	42.697	9.892	1.00	22.75
2071	CD1	TYR	A	464	22.563	41.933	9.758	1.00	23.07
2072	CE1	TYR	A	464	22.712	41.029	8.703	1.00	22.58

2073	CD2	TYR	A	464	20.397	42.538	8.943	1.00	23.44
2074	CE2	TYR	A	464	20.537	41.644	7.893	1.00	20.95
2075	CZ	TYR	A	464	21.692	40.894	7.779	1.00	22.05
2076	OH	TYR	A	464	21.819	40.001	6.744	1.00	21.31
2077	C	TYR	A	464	21.608	43.827	13.523	1.00	27.80
2078	O	TYR	A	464	22.803	44.064	13.685	1.00	28.04
2079	N	ARG	A	465	20.661	44.350	14.294	1.00	29.91
2080	CA	ARG	A	465	21.002	45.238	15.403	1.00	33.29
2081	CB	ARG	A	465	19.731	45.764	16.074	1.00	35.76
2082	CG	ARG	A	465	19.978	46.538	17.368	1.00	38.99
2083	CD	ARG	A	465	18.669	47.023	17.976	1.00	42.46
2084	NE	ARG	A	465	18.868	47.706	19.252	1.00	44.44
2085	CZ	ARG	A	465	17.897	48.297	19.943	1.00	46.85
2086	NH1	ARG	A	465	16.652	48.294	19.482	1.00	47.83
2087	NH2	ARG	A	465	18.167	48.890	21.097	1.00	47.38
2088	C	ARG	A	465	21.858	44.503	16.436	1.00	34.75
2089	O	ARG	A	465	21.406	43.540	17.055	1.00	34.47
2090	N	ASP	A	466	23.095	44.961	16.608	1.00	36.62
2091	CA	ASP	A	466	24.026	44.372	17.569	1.00	38.83
2092	CB	ASP	A	466	23.456	44.470	18.988	1.00	39.46
2093	CG	ASP	A	466	23.231	45.902	19.429	1.00	40.61
2094	OD1	ASP	A	466	24.151	46.729	19.242	1.00	40.51
2095	OD2	ASP	A	466	22.141	46.198	19.968	1.00	40.94
2096	C	ASP	A	466	24.407	42.921	17.288	1.00	39.96
2097	O	ASP	A	466	24.783	42.187	18.203	1.00	39.85
2098	N	MET	A	467	24.311	42.500	16.031	1.00	41.66
2099	CA	MET	A	467	24.674	41.132	15.678	1.00	43.69
2100	CB	MET	A	467	24.328	40.841	14.217	1.00	43.01
2101	CG	MET	A	467	24.631	39.416	13.797	1.00	43.53
2102	SD	MET	A	467	24.328	39.125	12.053	1.00	45.18
2103	CE	MET	A	467	22.544	38.865	12.066	1.00	44.23
2104	C	MET	A	467	26.175	40.966	15.889	1.00	45.56
2105	O	MET	A	467	26.619	40.175	16.722	1.00	46.26

2106	N	TYR	A	468	26.950	41.724	15.122	1.00	46.99
2107	CA	TYR	A	468	28.403	41.691	15.215	1.00	48.84
2108	CB	TYR	A	468	29.016	41.118	13.930	1.00	48.71
2109	CG	TYR	A	468	28.731	39.646	13.712	1.00	48.95
2110	CD1	TYR	A	468	27.913	39.218	12.665	1.00	49.23
2111	CE1	TYR	A	468	27.644	37.861	12.468	1.00	49.07
2112	CD2	TYR	A	468	29.273	38.680	14.560	1.00	49.57
2113	CE2	TYR	A	468	29.011	37.324	14.374	1.00	49.37
2114	CZ	TYR	A	468	28.197	36.921	13.328	1.00	49.98
2115	OH	TYR	A	468	27.940	35.580	13.147	1.00	49.98
2116	C	TYR	A	468	28.928	43.101	15.462	1.00	49.62
2117	O	TYR	A	468	29.141	43.829	14.472	1.00	50.21
2118	OT	TYR	A	468	29.091	43.471	16.646	1.00	50.66
2119	CB	GLU	B	685	18.548	43.302	21.979	1.00	63.65
2120	CG	GLU	B	685	18.317	43.165	23.475	1.00	63.87
2121	CD	GLU	B	685	18.479	41.737	23.956	1.00	64.23
2122	OE1	GLU	B	685	17.606	40.903	23.635	1.00	64.28
2123	OE2	GLU	B	685	19.478	41.445	24.647	1.00	64.53
2124	C	GLU	B	685	16.486	44.447	21.144	1.00	61.94
2125	O	GLU	B	685	15.986	44.713	20.050	1.00	62.27
2126	N	GLU	B	685	18.323	45.755	22.227	1.00	62.90
2127	CA	GLU	B	685	17.990	44.588	21.363	1.00	62.73
2128	N	ARG	B	686	15.773	44.020	22.185	1.00	60.58
2129	CA	ARG	B	686	14.324	43.847	22.118	1.00	59.13
2130	CB	ARG	B	686	13.677	45.103	21.527	1.00	60.07
2131	CG	ARG	B	686	12.155	45.100	21.495	1.00	61.27
2132	CD	ARG	B	686	11.558	45.589	22.807	1.00	62.16
2133	NE	ARG	B	686	10.176	46.030	22.634	1.00	63.43
2134	CZ	ARG	B	686	9.159	45.223	22.350	1.00	64.44
2135	NH1	ARG	B	686	9.361	43.920	22.210	1.00	64.89
2136	NH2	ARG	B	686	7.940	45.722	22.188	1.00	65.34
2137	C	ARG	B	686	13.919	42.623	21.291	1.00	57.39
2138	O	ARG	B	686	13.657	41.552	21.841	1.00	58.48

2139	N	HIS	B	687	13.874	42.792	19.972	1.00	54.71
2140	CA	HIS	B	687	13.488	41.724	19.049	1.00	51.16
2141	CB	HIS	B	687	14.325	40.462	19.290	1.00	51.72
2142	CG	HIS	B	687	15.785	40.639	19.009	1.00	51.47
2143	CD2	HIS	B	687	16.566	40.153	18.016	1.00	51.61
2144	ND1	HIS	B	687	16.608	41.410	19.801	1.00	52.04
2145	CE1	HIS	B	687	17.834	41.390	19.308	1.00	51.83
2146	NE2	HIS	B	687	17.835	40.635	18.225	1.00	51.34
2147	C	HIS	B	687	12.008	41.392	19.204	1.00	48.80
2148	O	HIS	B	687	11.637	40.237	19.403	1.00	48.44
2149	N	ALA	B	688	11.168	42.417	19.100	1.00	45.79
2150	CA	ALA	B	688	9.725	42.258	19.240	1.00	43.75
2151	CB	ALA	B	688	9.041	43.614	19.092	1.00	43.70
2152	C	ALA	B	688	9.115	41.263	18.255	1.00	41.94
2153	O	ALA	B	688	8.490	40.284	18.661	1.00	40.94
2154	N	ILE	B	689	9.295	41.517	16.963	1.00	40.75
2155	CA	ILE	B	689	8.740	40.649	15.931	1.00	39.42
2156	CB	ILE	B	689	9.107	41.161	14.523	1.00	39.12
2157	CG2	ILE	B	689	8.638	40.169	13.463	1.00	38.63
2158	CG1	ILE	B	689	8.460	42.530	14.296	1.00	38.90
2159	CD1	ILE	B	689	8.741	43.134	12.937	1.00	39.20
2160	C	ILE	B	689	9.189	39.200	16.077	1.00	38.83
2161	O	ILE	B	689	8.367	38.282	16.048	1.00	37.60
2162	N	LEU	B	690	10.491	38.998	16.238	1.00	38.40
2163	CA	LEU	B	690	11.033	37.656	16.393	1.00	38.63
2164	CB	LEU	B	690	12.548	37.730	16.597	1.00	39.36
2165	CG	LEU	B	690	13.382	36.561	16.069	1.00	40.30
2166	CD1	LEU	B	690	14.860	36.928	16.113	1.00	39.81
2167	CD2	LEU	B	690	13.108	35.314	16.889	1.00	41.50
2168	C	LEU	B	690	10.358	36.989	17.593	1.00	39.78
2169	O	LEU	B	690	9.895	35.850	17.505	1.00	38.83
2170	N	HIS	B	691	10.294	37.706	18.713	1.00	40.27
2171	CA	HIS	B	691	9.647	37.176	19.911	1.00	41.72

2172	CB	HIS	B	691	9.668	38.211	21.036	1.00	43.49
2173	CG	HIS	B	691	10.897	38.155	21.887	1.00	45.34
2174	CD2	HIS	B	691	11.909	39.040	22.053	1.00	46.24
2175	ND1	HIS	B	691	11.186	37.085	22.705	1.00	46.60
2176	CE1	HIS	B	691	12.322	37.313	23.339	1.00	46.83
2177	NE2	HIS	B	691	12.781	38.492	22.962	1.00	47.22
2178	C	HIS	B	691	8.205	36.799	19.596	1.00	41.36
2179	O	HIS	B	691	7.741	35.717	19.959	1.00	41.77
2180	N	ARG	B	692	7.502	37.698	18.915	1.00	40.51
2181	CA	ARG	B	692	6.112	37.459	18.543	1.00	40.58
2182	CB	ARG	B	692	5.588	38.617	17.692	1.00	41.97
2183	CG	ARG	B	692	4.108	38.532	17.339	1.00	44.31
2184	CD	ARG	B	692	3.755	39.573	16.287	1.00	46.39
2185	NE	ARG	B	692	4.450	39.308	15.029	1.00	48.87
2186	CZ	ARG	B	692	4.516	40.159	14.010	1.00	49.52
2187	NH1	ARG	B	692	3.929	41.346	14.093	1.00	50.67
2188	NH2	ARG	B	692	5.172	39.822	12.907	1.00	49.63
2189	C	ARG	B	692	5.998	36.152	17.760	1.00	39.77
2190	O	ARG	B	692	5.250	35.252	18.148	1.00	38.70
2191	N	LEU	B	693	6.746	36.052	16.663	1.00	38.99
2192	CA	LEU	B	693	6.730	34.854	15.825	1.00	39.44
2193	CB	LEU	B	693	7.812	34.932	14.741	1.00	38.36
2194	CG	LEU	B	693	7.643	35.944	13.604	1.00	38.71
2195	CD1	LEU	B	693	8.848	35.865	12.684	1.00	37.17
2196	CD2	LEU	B	693	6.365	35.657	12.828	1.00	37.74
2197	C	LEU	B	693	6.936	33.587	16.641	1.00	40.12
2198	O	LEU	B	693	6.290	32.569	16.399	1.00	40.20
2199	N	LEU	B	694	7.842	33.651	17.609	1.00	41.30
2200	CA	LEU	B	694	8.125	32.498	18.450	1.00	43.03
2201	CB	LEU	B	694	9.406	32.740	19.250	1.00	41.27
2202	CG	LEU	B	694	10.694	32.762	18.421	1.00	40.09
2203	CD1	LEU	B	694	11.853	33.242	19.269	1.00	39.04
2204	CD2	LEU	B	694	10.964	31.366	17.874	1.00	39.24

2205	C	LEU	B	694	6.974	32.178	19.399	1.00	45.64
2206	O	LEU	B	694	6.877	31.061	19.905	1.00	44.78
2207	N	GLN	B	695	6.099	33.153	19.628	1.00	49.29
2208	CA	GLN	B	695	4.967	32.964	20.532	1.00	53.51
2209	CB	GLN	B	695	4.350	34.316	20.912	1.00	53.94
2210	CG	GLN	B	695	5.336	35.354	21.441	1.00	54.96
2211	CD	GLN	B	695	6.069	34.916	22.699	1.00	55.61
2212	OE1	GLN	B	695	6.860	35.677	23.263	1.00	55.52
2213	NE2	GLN	B	695	5.814	33.690	23.144	1.00	55.62
2214	C	GLN	B	695	3.873	32.061	19.959	1.00	55.94
2215	O	GLN	B	695	3.035	31.553	20.702	1.00	55.76
2216	N	GLU	B	696	3.880	31.866	18.644	1.00	58.97
2217	CA	GLU	B	696	2.882	31.025	17.984	1.00	62.61
2218	CB	GLU	B	696	1.467	31.515	18.320	1.00	63.02
2219	CG	GLU	B	696	1.294	33.044	18.453	1.00	63.82
2220	CD	GLU	B	696	1.649	33.832	17.202	1.00	64.13
2221	OE1	GLU	B	696	1.115	33.519	16.115	1.00	64.51
2222	OE2	GLU	B	696	2.454	34.777	17.309	1.00	64.16
2223	C	GLU	B	696	3.055	31.054	16.473	1.00	64.98
2224	O	GLU	B	696	2.671	30.129	15.756	1.00	65.58
2225	N	GLY	B	697	3.643	32.150	16.021	1.00	67.35
2226	CA	GLY	B	697	3.875	32.400	14.618	1.00	70.03
2227	C	GLY	B	697	3.612	33.876	14.561	1.00	71.80
2228	O	GLY	B	697	3.004	34.366	13.584	1.00	71.76
2229	OT	GLY	B	697	4.003	34.560	15.534	1.00	71.76
2230	O	HOH	S	1	23.021	22.410	-2.190	1.00	19.60
2231	O	HOH	S	2	16.829	36.197	0.666	1.00	18.07
2232	O	HOH	S	3	22.165	35.434	11.145	1.00	15.63
2233	O	HOH	S	4	24.975	20.256	-2.262	1.00	20.14
2234	O	HOH	S	5	22.159	29.605	15.803	1.00	19.70
2235	O	HOH	S	6	24.989	31.512	-0.644	1.00	16.40
2236	O	HOH	S	7	10.834	33.694	-3.352	1.00	17.23
2237	O	HOH	S	8	22.460	38.715	-17.965	1.00	31.92

2238	O	HOH	S	9	17.528	31.039	1.273	1.00	14.10
2239	O	HOH	S	10	29.026	37.829	2.231	1.00	16.59
2240	O	HOH	S	11	16.137	33.624	0.850	1.00	17.71
2241	O	HOH	S	12	21.555	23.965	-0.430	1.00	13.97
2242	O	HOH	S	13	24.577	41.484	-5.877	1.00	19.10
2243	O	HOH	S	14	34.344	22.171	2.655	1.00	23.28
2244	O	HOH	S	15	23.968	19.698	-6.030	1.00	21.97
2245	O	HOH	S	16	12.341	31.084	-5.780	1.00	18.26
2246	O	HOH	S	17	17.291	24.202	0.490	1.00	21.48
2247	O	HOH	S	18	12.775	35.658	-4.277	1.00	15.87
2248	O	HOH	S	19	32.945	42.649	9.747	1.00	47.61
2249	O	HOH	S	20	6.636	45.304	0.256	1.00	32.40
2250	O	HOH	S	21	11.642	46.359	3.122	1.00	47.12
2251	O	HOH	S	22	15.366	32.455	-1.716	1.00	24.92
2252	O	HOH	S	23	15.186	49.092	-1.355	1.00	26.79
2253	O	HOH	S	24	17.321	27.755	27.447	1.00	23.87
2254	O	HOH	S	25	32.119	32.883	-0.957	1.00	24.24
2255	O	HOH	S	26	17.226	13.378	7.046	1.00	30.98
2256	O	HOH	S	27	17.607	52.477	-12.562	1.00	30.41
2257	O	HOH	S	28	11.582	28.462	0.833	1.00	27.74
2258	O	HOH	S	29	29.336	58.175	3.211	1.00	24.47
2259	O	HOH	S	30	20.328	34.102	24.740	1.00	27.25
2260	O	HOH	S	31	11.297	30.724	-3.163	1.00	29.15
2261	O	HOH	S	32	14.539	17.647	-8.907	1.00	23.07
2262	O	HOH	S	33	12.598	30.559	30.560	1.00	24.86
2263	O	HOH	S	34	5.025	18.187	3.778	1.00	28.69
2264	O	HOH	S	35	14.927	26.075	0.820	1.00	31.48
2265	O	HOH	S	36	26.367	38.413	-9.182	1.00	23.21
2266	O	HOH	S	37	30.494	11.197	5.944	1.00	32.46
2267	O	HOH	S	38	11.293	49.824	6.074	1.00	48.93
2268	O	HOH	S	39	20.529	16.901	-4.931	1.00	32.28
2269	O	HOH	S	40	24.843	35.083	-15.519	1.00	21.88
2270	O	HOH	S	41	7.674	40.665	3.297	1.00	37.33

2271	O	HOH	S	42	27.523	46.282	-18.345	1.00	37.96
2272	O	HOH	S	43	22.709	13.774	-4.567	1.00	49.60
2273	O	HOH	S	44	7.423	32.242	11.910	1.00	23.05
2274	O	HOH	S	45	31.276	40.964	1.308	1.00	31.68
2275	O	HOH	S	46	33.265	32.328	3.517	1.00	19.13
2276	O	HOH	S	47	6.555	16.927	5.904	1.00	23.85
2277	O	HOH	S	48	17.606	50.658	7.865	1.00	28.11
2278	O	HOH	S	49	20.830	9.388	10.713	1.00	28.29
2279	O	HOH	S	50	13.364	37.050	29.629	1.00	23.94
2280	O	HOH	S	51	9.192	18.836	-1.960	1.00	33.23
2281	O	HOH	S	52	23.567	48.701	-14.763	1.00	55.81
2282	O	HOH	S	53	33.968	34.742	2.852	1.00	26.86
2283	O	HOH	S	54	29.820	10.990	8.338	1.00	28.51
2284	O	HOH	S	55	11.748	42.238	23.648	1.00	42.57
2285	O	HOH	S	56	14.767	33.631	-4.195	1.00	32.75
2286	O	HOH	S	57	12.500	34.343	29.890	1.00	22.65
2287	O	HOH	S	58	28.117	41.866	-15.415	1.00	31.74
2288	O	HOH	S	59	26.356	40.551	-7.512	1.00	22.73
2289	O	HOH	S	60	22.268	46.641	-15.890	1.00	50.83
2290	O	HOH	S	61	7.181	15.455	0.062	1.00	44.46
2291	O	HOH	S	62	3.620	30.584	-0.194	1.00	36.39
2292	O	HOH	S	63	6.128	27.849	3.787	1.00	52.56
2293	O	HOH	S	64	31.099	55.471	8.227	1.00	30.35
2294	O	HOH	S	65	18.603	58.163	-1.009	1.00	47.14
2295	O	HOH	S	66	8.356	23.629	26.974	1.00	32.72
2296	O	HOH	S	67	19.654	57.594	-3.383	1.00	43.61
2297	O	HOH	S	68	20.930	28.296	33.352	1.00	40.59
2298	O	HOH	S	69	21.652	36.732	27.720	1.00	35.00
2299	O	HOH	S	70	31.556	42.782	3.272	1.00	30.88
2300	O	HOH	S	71	13.327	50.293	2.487	1.00	38.75
2301	O	HOH	S	72	19.141	53.232	5.426	1.00	37.22
2302	O	HOH	S	73	10.869	22.357	19.472	1.00	19.26
2303	O	HOH	S	74	4.005	20.489	2.211	1.00	37.71

2304	O	HOH	S	75	32.792	10.675	9.182	1.00	22.60
2305	O	HOH	S	76	15.967	27.450	-1.311	1.00	30.63
2306	O	HOH	S	77	6.796	41.276	9.965	1.00	45.09
2307	O	HOH	S	78	6.261	30.440	7.929	1.00	33.02
2308	O	HOH	S	79	19.308	14.907	21.667	1.00	42.45
2309	O	HOH	S	80	2.565	29.418	1.814	1.00	40.89
2310	O	HOH	S	81	2.180	49.135	-16.647	1.00	53.37
2311	O	HOH	S	82	36.343	8.679	3.325	1.00	40.82
2312	O	HOH	S	83	22.711	19.517	29.686	1.00	47.69
2313	O	HOH	S	84	33.973	34.630	0.258	1.00	31.56
2314	O	HOH	S	85	31.745	38.264	1.536	1.00	22.56
2315	O	HOH	S	86	5.827	37.873	6.417	1.00	48.05
2316	O	HOH	S	87	19.499	17.423	-8.991	1.00	38.26
2317	O	HOH	S	88	40.418	35.587	7.944	1.00	35.76
2318	O	HOH	S	89	15.390	46.880	15.780	1.00	39.90
2319	O	HOH	S	90	6.878	29.542	-13.424	1.00	40.19
2320	O	HOH	S	91	8.647	28.612	20.656	1.00	29.73
2321	O	HOH	S	92	22.042	37.435	22.086	1.00	37.50
2322	O	HOH	S	93	27.585	30.929	23.977	1.00	32.74
2323	O	HOH	S	94	10.974	31.175	27.894	1.00	24.96
2324	O	HOH	S	95	26.202	25.474	-11.896	1.00	41.41
2325	O	HOH	S	96	6.726	33.443	-14.585	1.00	36.10
2326	O	HOH	S	97	15.550	8.924	10.717	1.00	33.88
2327	O	HOH	S	98	16.476	16.841	-2.591	1.00	26.55
2328	O	HOH	S	99	28.319	28.274	12.336	1.00	43.77
2329	O	HOH	S	100	27.769	3.457	13.155	1.00	48.23
2330	O	HOH	S	101	24.882	39.541	-19.201	1.00	53.25
2331	O	HOH	S	102	12.968	44.583	-8.525	1.00	25.37
2332	O	HOH	S	103	20.637	61.548	2.038	1.00	57.43
2333	O	HOH	S	104	18.394	21.172	-12.670	1.00	30.69
2334	O	HOH	S	105	21.685	40.720	28.499	1.00	31.23
2335	O	HOH	S	106	37.452	24.342	8.575	1.00	43.15
2336	O	HOH	S	107	28.072	12.030	-2.850	1.00	35.13

2337	O	HOH	S	108	13.643	6.793	9.813	1.00	59.43
2338	O	HOH	S	109	29.194	47.369	-11.513	1.00	33.93
2339	O	HOH	S	110	37.211	25.400	11.266	1.00	49.29
2340	O	HOH	S	111	32.452	24.117	12.117	1.00	37.91
2341	O	HOH	S	112	20.047	18.433	-15.782	1.00	52.69
2342	O	HOH	S	113	37.297	36.567	3.622	1.00	50.95
2343	O	HOH	S	114	26.638	37.932	27.578	1.00	60.19
2344	O	HOH	S	115	40.067	37.141	6.034	1.00	62.83
2345	O	HOH	S	116	16.702	28.787	32.709	1.00	45.22
2346	O	HOH	S	117	15.614	14.400	-2.970	1.00	32.52
2347	O	HOH	S	118	25.304	43.389	12.324	1.00	46.21
2348	O	HOH	S	119	35.986	27.446	-0.047	1.00	39.51
2349	O	HOH	S	120	33.667	38.724	-6.920	1.00	55.40
2350	O	HOH	S	121	2.653	22.799	6.024	1.00	32.62
2351	O	HOH	S	122	21.427	16.319	32.924	1.00	56.84
2352	O	HOH	S	123	-2.535	25.653	7.482	1.00	49.14
2353	O	HOH	S	124	38.296	26.623	7.497	1.00	36.28
2354	O	HOH	S	125	24.325	56.054	-3.208	1.00	42.51
2355	O	HOH	S	126	31.374	39.772	-15.850	1.00	43.44
2356	O	HOH	S	127	14.293	49.969	9.738	1.00	46.86
2357	O	HOH	S	128	29.446	46.358	-15.130	1.00	56.58
2358	O	HOH	S	129	13.234	46.587	14.294	1.00	30.39
2359	O	HOH	S	130	28.696	21.460	14.541	1.00	43.43
2360	O	HOH	S	131	29.833	19.823	16.133	1.00	53.77
2361	O	HOH	S	132	28.668	40.610	0.027	1.00	27.60
2362	O	HOH	S	133	31.999	29.578	17.949	1.00	52.12
2363	O	HOH	S	134	32.331	41.291	-7.181	1.00	48.91
2364	O	HOH	S	135	18.143	37.552	22.925	1.00	31.27
2365	O	HOH	S	136	16.874	57.740	-7.181	1.00	36.07
2366	O	HOH	S	137	3.614	38.629	3.896	1.00	63.76
2367	O	HOH	S	138	18.541	13.341	-5.104	1.00	59.11
2368	O	HOH	S	139	6.118	51.002	-15.654	1.00	38.96
2369	O	HOH	S	140	14.730	25.982	29.459	1.00	32.23

2370	O	HOH	S	141	21.736	19.325	-8.319	1.00	36.70
2371	O	HOH	S	142	8.176	16.537	17.699	1.00	58.27
2372	O	HOH	S	143	11.696	32.975	0.495	1.00	36.22
2373	O	HOH	S	144	13.563	48.324	0.595	1.00	37.61
2374	O	HOH	S	145	12.379	12.447	17.047	1.00	62.89
2375	O	HOH	S	146	9.604	31.872	1.213	1.00	68.72
2376	O	HOH	S	147	28.144	19.163	18.746	1.00	42.30
2377	O	HOH	S	148	32.515	45.933	-7.466	1.00	37.61
2378	O	HOH	S	149	24.759	0.889	18.947	1.00	66.75
2379	O	HOH	S	150	39.683	22.653	2.230	1.00	35.42
2380	O	HOH	S	151	13.554	52.853	2.352	1.00	37.57
2381	O	HOH	S	152	8.318	48.977	2.507	1.00	73.06
2382	O	HOH	S	153	8.633	28.003	-12.609	1.00	33.91
2383	O	HOH	S	154	2.882	30.152	4.149	1.00	62.49
2384	O	HOH	S	155	31.535	7.386	4.692	1.00	35.95
2385	O	HOH	S	156	5.852	26.333	22.676	1.00	39.01
2386	O	HOH	S	157	7.617	46.335	-19.650	1.00	50.76
2387	O	HOH	S	158	23.004	9.857	-2.493	1.00	64.92
2388	O	HOH	S	159	6.680	37.243	8.927	1.00	35.74
2389	O	HOH	S	160	1.655	40.656	10.739	1.00	68.96
2390	O	HOH	S	161	37.861	28.017	11.079	1.00	29.28
2391	O	HOH	S	162	2.363	30.081	11.152	1.00	47.90
2392	O	HOH	S	163	22.816	6.883	24.251	1.00	50.27
2393	O	HOH	S	164	25.232	24.018	-9.509	1.00	56.25
2394	O	HOH	S	165	31.917	40.723	-4.749	1.00	43.99
2395	O	HOH	S	166	29.060	32.100	-14.160	1.00	48.37
2396	O	HOH	S	167	6.850	24.422	13.622	1.00	30.86
2397	O	HOH	S	168	31.128	26.378	-0.266	1.00	26.16
2398	O	HOH	S	169	26.393	4.775	16.316	1.00	46.62
2399	O	HOH	S	170	30.226	52.800	-0.982	1.00	62.86
2400	O	HOH	S	171	11.260	25.311	-15.954	1.00	30.67
2401	O	HOH	S	172	8.236	22.803	-8.257	1.00	36.47
2402	O	HOH	S	173	32.734	30.835	1.127	1.00	29.48

2403	O	HOH	S	174	12.162	13.528	-6.989	1.00	54.81
2404	O	HOH	S	175	10.004	18.589	-15.661	1.00	52.49
2405	O	HOH	S	176	2.597	15.841	3.847	1.00	36.47
2406	O	HOH	S	177	16.049	21.664	25.082	1.00	36.38
2407	O	HOH	S	178	9.566	53.021	5.395	1.00	51.65
2408	O	HOH	S	179	9.844	33.557	29.120	1.00	41.08
2409	O	HOH	S	180	28.907	9.505	-2.595	1.00	43.51
2410	O	HOH	S	181	29.014	14.102	-1.746	1.00	52.94
2411	O	HOH	S	182	8.615	16.558	11.985	1.00	34.51
2412	O	HOH	S	183	12.854	16.652	-1.111	1.00	38.29
2413	O	HOH	S	184	28.378	56.857	-0.308	1.00	70.56
2414	O	HOH	S	185	21.366	14.621	28.348	1.00	75.81
2415	O	HOH	S	186	29.539	7.952	13.215	1.00	47.28
2416	O	HOH	S	187	32.951	32.466	15.334	1.00	53.06
2417	O	HOH	S	188	6.055	23.083	15.885	1.00	44.59
2418	O	HOH	S	189	32.033	9.844	17.068	1.00	61.54
2419	O	HOH	S	190	31.234	15.535	16.608	1.00	47.53
2420	O	HOH	S	191	25.418	9.801	20.811	1.00	55.35
2421	O	HOH	S	192	17.915	17.399	-4.929	1.00	38.99
2422	O	HOH	S	193	20.092	56.578	-12.068	1.00	34.77
2423	O	HOH	S	194	5.198	29.909	5.015	1.00	54.91
2424	O	HOH	S	195	14.259	59.116	-6.790	1.00	57.78
2425	O	HOH	S	196	2.335	36.084	19.359	1.00	71.38
2426	O	HOH	S	197	25.907	29.027	30.690	1.00	45.68
2427	O	HOH	S	198	7.004	27.666	7.371	1.00	33.37
2428	O	HOH	S	199	29.917	10.266	3.633	1.00	28.69
2429	O	HOH	S	200	3.229	39.595	8.996	1.00	64.29
2430	O	HOH	S	201	11.658	26.014	31.457	1.00	30.92
2431	O	HOH	S	202	30.585	43.900	-10.316	1.00	35.47
2432	O	HOH	S	203	5.657	20.000	12.450	1.00	36.93
2433	O	HOH	S	204	9.001	8.083	12.525	1.00	44.27
2434	O	HOH	S	205	18.577	1.267	23.323	1.00	53.87
2435	O	HOH	S	206	14.129	50.521	-14.443	1.00	54.64

2436	O	HOH	S	207	18.959	15.493	28.375	1.00	71.59
2437	O	HOH	S	208	0.669	37.375	17.680	1.00	49.95
2438	O	HOH	S	209	26.872	55.578	-2.201	1.00	46.16
2439	O	HOH	S	210	6.168	22.883	11.718	1.00	31.87
2440	O	HOH	S	211	9.897	16.355	-1.729	1.00	36.68
2441	O	HOH	S	212	30.265	27.848	23.670	1.00	53.45
2442	O	HOH	S	213	30.762	47.558	-1.627	1.00	42.34
2443	O	HOH	S	214	32.189	35.014	15.024	1.00	44.29
2444	O	HOH	S	215	10.272	34.635	-0.779	1.00	25.15
2445	O	HOH	S	216	4.890	17.836	16.021	1.00	58.71
2446	O	HOH	S	217	5.733	41.605	7.246	1.00	41.48
2447	O	HOH	S	218	24.986	27.076	-7.629	1.00	61.37
2448	O	HOH	S	219	26.433	10.728	26.102	1.00	47.70
2449	O	HOH	S	220	9.403	26.411	28.194	1.00	51.51
2450	O	HOH	S	221	22.508	23.957	-9.377	1.00	43.79
2451	O	HOH	S	222	36.297	31.156	7.134	1.00	49.35
2452	O	HOH	S	223	16.073	56.555	4.729	1.00	47.51
2453	O	HOH	S	224	9.102	45.988	15.199	1.00	51.54
2454	O	HOH	S	225	22.868	15.999	-6.862	1.00	48.61
2455	O	HOH	S	226	4.554	37.721	10.138	1.00	63.61
2456	O	HOH	S	227	8.317	20.227	-8.684	1.00	40.62
2457	O	HOH	S	228	26.553	17.081	26.527	1.00	60.48
2458	O	HOH	S	229	18.435	52.120	-15.938	1.00	68.74
2459	O	HOH	S	230	15.731	11.256	6.138	1.00	40.27
2460	O	HOH	S	231	-2.470	33.671	15.319	1.00	56.63
2461	O	HOH	S	232	9.235	37.391	27.202	1.00	50.70
2462	O	HOH	S	233	22.857	5.454	-0.374	1.00	56.93
2463	O	HOH	S	234	1.412	28.065	19.093	1.00	54.97
2464	O	HOH	S	235	29.383	5.654	12.365	1.00	46.23
2465	O	HOH	S	236	21.394	2.024	21.053	1.00	54.78
2466	O	HOH	S	237	3.134	52.176	-19.288	1.00	61.95
2467	O	HOH	S	238	22.005	57.555	-0.605	1.00	48.17
2468	O	HOH	S	239	13.682	3.617	13.009	1.00	43.82

2469	O	HOH	S	240	19.176	16.596	19.466	1.00	31.39
2470	O	HOH	S	241	3.338	33.539	6.594	1.00	47.67
2471	O	HOH	S	242	10.760	2.995	19.481	1.00	70.14
2472	O	HOH	S	243	16.801	17.522	20.526	1.00	63.73
2473	O	HOH	S	244	2.600	44.637	16.700	1.00	56.53
2474	O	HOH	S	245	27.872	14.286	18.168	1.00	41.98
2475	O	HOH	S	246	31.396	45.519	-13.517	1.00	53.59
2476	O	HOH	S	247	31.244	35.576	-11.964	1.00	33.65
2477	O	HOH	S	248	21.693	4.459	26.360	1.00	52.63
2478	O	HOH	S	249	10.433	20.471	21.568	1.00	35.08
2479	O	HOH	S	250	17.785	18.041	18.016	1.00	49.80
2480	O	HOH	S	251	12.908	41.185	25.864	1.00	49.78
2481	O	HOH	S	252	11.825	38.262	27.686	1.00	41.47
2482	O	HOH	S	253	21.717	14.484	25.654	1.00	49.41
2483	O	HOH	S	254	3.264	19.434	-21.232	1.00	58.93
2484	O	HOH	S	255	32.144	44.531	-1.765	1.00	63.10
2485	O	HOH	S	256	30.528	19.733	26.321	1.00	56.72
2486	O	HOH	S	257	1.014	38.169	8.350	1.00	69.65
2487	O	HOH	S	258	15.650	56.451	-11.110	1.00	45.85
2488	O	HOH	S	259	9.637	49.206	-12.734	1.00	31.76
2489	O	HOH	S	260	26.271	33.962	11.972	1.00	28.74
2490	O	HOH	S	261	16.265	55.388	-6.013	1.00	48.50
2491	O	HOH	S	262	35.225	25.151	1.974	1.00	37.37
2492	O	HOH	S	263	34.131	31.093	10.695	1.00	35.88
2493	O	HOH	S	264	9.808	12.096	-10.102	1.00	42.96
2494	O	HOH	S	265	31.337	17.800	15.541	1.00	54.02
2495	O	HOH	S	266	6.034	17.605	1.265	1.00	32.48
2496	O	HOH	S	267	10.657	28.653	26.815	1.00	33.27
2497	O	HOH	S	268	33.123	28.220	0.778	1.00	32.26
2498	O	HOH	S	269	4.688	49.518	-17.401	1.00	56.01
2499	O	HOH	S	270	19.934	38.276	25.088	1.00	52.01
2500	O	HOH	S	271	17.067	16.746	-7.685	1.00	44.99
2501	O	HOH	S	272	8.184	32.997	31.099	1.00	38.13

2502	O	HOH	S	273	15.358	23.005	31.926	1.00	47.35
2503	O	HOH	S	274	37.594	33.163	10.831	1.00	50.51
2504	O	HOH	S	275	26.340	26.057	14.475	1.00	43.81
2505	O	HOH	S	276	9.314	11.770	3.305	1.00	52.95
2506	O	HOH	S	277	29.890	5.053	4.222	1.00	39.94
2507	O	HOH	S	278	21.596	63.668	5.719	1.00	47.51
2508	O	HOH	S	280	4.234	31.186	9.139	1.00	34.04
2509	O	HOH	S	281	20.211	52.099	-12.173	1.00	32.14
2510	O	HOH	S	282	31.764	46.901	-9.886	1.00	37.63
2511	O	HOH	S	283	29.356	16.377	18.834	1.00	47.88
2512	O	HOH	S	284	7.077	22.502	23.360	1.00	49.62
2513	O	HOH	S	285	10.457	17.845	24.918	1.00	45.38
2514	O	HOH	S	286	22.709	21.642	-7.858	1.00	44.54
2515	O	HOH	S	287	41.743	38.399	4.312	1.00	51.42
2516	O	HOH	S	288	28.342	29.192	29.846	1.00	35.37
2517	O	HOH	S	289	19.871	8.666	8.338	1.00	36.88
2518	O	HOH	S	290	30.239	47.828	14.437	1.00	52.48
2519	O	HOH	S	291	38.133	31.699	-0.085	1.00	48.80
2520	O	HOH	S	292	29.451	19.522	21.988	1.00	48.53
2521	O	HOH	S	293	28.207	17.784	23.529	1.00	49.19
2522	O	HOH	S	294	25.099	25.880	30.696	1.00	50.04
2523	O	HOH	S	295	20.984	24.305	-13.635	1.00	35.02
2524	O	HOH	S	296	27.314	9.229	14.571	1.00	37.16
2525	O	HOH	S	297	5.590	44.198	15.517	1.00	46.00
2526	O	HOH	S	298	1.452	15.832	16.496	1.00	48.72
2527	O	HOH	S	299	31.895	52.120	-9.294	1.00	36.65
2528	O	HOH	S	300	2.789	26.865	21.392	1.00	37.83
2529	O	HOH	S	301	10.822	21.853	1.469	1.00	38.42
2530	O	HOH	S	302	25.182	43.665	22.197	1.00	39.85
2531	O	HOH	S	303	10.013	44.307	3.131	1.00	61.53
2532	O	HOH	S	304	25.076	12.353	-5.192	1.00	49.90
2533	O	HOH	S	305	24.684	26.059	34.224	1.00	51.37
2534	O	HOH	S	306	17.636	17.778	-11.960	1.00	54.01

2535	O	HOH	S	307	21.679	9.218	-4.605	1.00	50.75
2536	O	HOH	S	308	12.832	30.478	-0.749	1.00	46.31
2537	O	HOH	S	309	-0.832	31.716	16.046	1.00	49.15
2538	O	HOH	S	310	11.345	25.092	29.161	1.00	54.91
2539	O	HOH	S	311	38.438	33.351	4.404	1.00	47.87
2540	O	HOH	S	312	29.760	48.475	-20.473	1.00	61.21
2541	O	HOH	S	313	19.889	22.967	34.487	1.00	53.69
2542	O	HOH	S	314	6.167	6.357	12.405	1.00	45.47
2543	O	HOH	S	315	24.800	24.028	-13.646	1.00	41.36
2544	O	HOH	S	316	34.408	33.833	13.704	1.00	48.67
2545	O	HOH	S	317	28.499	24.877	15.179	1.00	42.44
2546	O	HOH	S	318	18.760	10.026	-0.303	1.00	47.49
2547	O	HOH	S	319	27.889	33.343	15.965	1.00	46.60
2548	O	HOH	S	320	28.099	54.149	-9.913	1.00	47.31
2549	O	HOH	S	321	6.669	20.044	17.321	1.00	66.41
2550	O	HOH	S	322	9.183	51.425	-1.061	1.00	50.92
2551	O	HOH	S	323	26.136	49.957	-13.069	1.00	44.73
2552	O	HOH	S	324	6.462	14.964	10.693	1.00	50.61
2553	O	HOH	S	325	27.434	21.342	29.941	1.00	46.70
2554	O	HOH	S	326	-2.372	39.018	9.502	1.00	48.95
2555	O	HOH	S	327	39.676	34.723	11.054	1.00	54.77
2556	O	HOH	S	328	31.515	4.167	11.728	1.00	38.27
2557	O	HOH	S	329	30.273	43.414	12.468	1.00	56.22
2558	O	HOH	S	330	31.821	6.860	14.047	1.00	49.62
2559	O	HOH	S	331	34.176	36.382	-11.484	1.00	54.81
2560	O	HOH	S	332	16.341	29.905	-0.825	1.00	50.86
2561	O	HOH	S	333	16.034	14.050	-0.096	1.00	26.81
2562	O	HOH	S	334	35.569	39.304	6.909	1.00	58.70
2563	O	HOH	S	335	7.222	18.767	-13.380	1.00	48.09
2564	O	HOH	S	336	4.343	25.758	17.613	1.00	48.32
2565	O	HOH	S	337	23.980	49.898	20.317	1.00	45.46
2566	O	HOH	S	338	-1.308	39.173	20.570	1.00	47.06
2567	O	HOH	S	339	29.401	35.057	-13.568	1.00	51.53

2568	O	HOH	S	340	22.171	11.944	-8.266	1.00	58.38
2569	O	HOH	S	341	28.556	23.420	-8.393	1.00	38.50
2570	O	HOH	S	342	16.039	7.600	25.055	1.00	63.84
2571	O	HOH	S	343	2.335	34.042	2.843	1.00	52.94
2572	O	HOH	S	344	14.874	19.553	25.906	1.00	44.98
2573	O	HOH	S	345	33.947	47.332	-12.606	1.00	52.85
2574	O	HOH	S	346	27.488	24.767	30.391	1.00	48.33
2575	O	HOH	S	347	20.467	43.261	26.119	1.00	52.94
2576	O	HOH	S	348	28.263	37.781	30.518	1.00	62.99
2577	O	HOH	S	349	27.485	34.119	-15.359	1.00	50.71
2578	O	HOH	S	350	25.657	34.532	30.427	1.00	54.08
2579	O	HOH	S	351	29.768	1.154	1.312	1.00	59.34
2580	O	HOH	S	352	5.457	39.028	22.172	1.00	47.10
2581	O	HOH	S	353	5.067	16.762	20.070	1.00	60.26
2582	O	HOH	S	354	18.638	55.700	-4.851	1.00	55.62
2583	O	HOH	S	355	32.686	59.039	10.830	1.00	39.90
2584	O	HOH	S	356	28.255	51.067	-11.879	1.00	52.57
2585	O	HOH	S	357	11.617	51.221	-1.789	1.00	63.06
2586	O	HOH	S	358	2.982	19.431	-24.499	1.00	45.57
2587	O	HOH	S	359	22.096	60.033	-1.451	1.00	61.45
2588	O	HOH	S	360	22.637	43.238	31.026	1.00	47.28
2589	O	HOH	S	361	30.447	38.954	29.873	1.00	57.25
2590	O	HOH	S	362	35.833	38.025	1.980	1.00	61.81
2591	O	HOH	S	363	6.113	31.893	-17.272	1.00	49.61
2592	O	HOH	S	364	6.724	15.601	-22.408	1.00	59.42
2593	O	HOH	S	365	12.111	1.178	18.316	1.00	48.35
2594	O	HOH	S	366	4.240	32.098	1.799	1.00	44.18
2595	O	HOH	S	367	29.724	35.065	27.753	1.00	55.76
2596	O	HOH	S	368	26.360	7.462	25.028	1.00	51.90
2597	O	HOH	S	369	9.107	46.874	3.890	1.00	56.70
2598	O	HOH	S	370	10.650	46.430	-20.344	1.00	37.21
2599	O	HOH	S	371	8.233	48.961	17.197	1.00	59.01
2600	O	HOH	S	372	20.322	15.007	-8.818	1.00	55.36

2601	O	HOH	S	373	19.260	-0.126	16.569	1.00	45.30
2602	O	HOH	S	374	7.343	49.778	-0.668	1.00	55.02
2603	O	HOH	S	375	2.507	47.867	0.719	1.00	48.12
2604	O	HOH	S	376	13.136	54.591	-2.145	1.00	53.44
2605	O	HOH	S	377	17.466	16.519	30.208	1.00	49.11
2606	O	HOH	S	378	20.118	10.769	23.252	1.00	55.34
2607	O	HOH	S	379	23.542	12.685	26.089	1.00	62.62
2608	O	HOH	S	380	20.375	47.120	12.159	1.00	51.92
2609	O	HOH	S	381	9.032	10.924	17.726	1.00	57.21
2610	O	HOH	S	382	15.077	15.226	30.470	1.00	56.74
2611	O	HOH	S	383	27.823	7.313	-8.539	1.00	49.75
2612	O	HOH	S	384	-1.210	31.371	18.699	1.00	53.14
2613	O	HOH	S	385	7.322	35.525	28.034	1.00	61.44
2614	O	HOH	S	386	14.217	16.674	-13.221	1.00	42.98
2615	O	HOH	S	387	20.078	59.930	-2.925	1.00	54.66
2616	O	HOH	S	388	28.936	2.000	15.009	1.00	47.04
2617	O	HOH	S	389	14.166	28.692	31.577	1.00	59.65
2618	O	HOH	S	390	20.846	52.499	14.026	1.00	61.68
2619	O	HOH	S	391	13.294	5.368	25.444	1.00	52.09
2620	O	HOH	S	392	26.874	59.625	-2.846	1.00	46.54
2621	O	HOH	S	393	11.393	5.392	16.760	1.00	45.29
2622	O	HOH	S	394	30.608	57.650	11.108	1.00	63.95
2623	O	HOH	S	395	33.858	39.183	-13.250	1.00	54.28
2624	O	HOH	S	396	16.117	14.396	-7.011	1.00	46.14
2625	O	HOH	S	397	37.725	38.263	6.165	1.00	64.28
2626	O	HOH	S	398	6.555	42.050	-19.474	1.00	48.56
2627	C1A	735	C	1	19.341	40.726	3.997	1.00	15.91
2628	O1C	735	C	1	18.234	40.214	4.328	1.00	17.26
2629	O1B	735	C	1	20.387	40.473	4.647	1.00	17.17
2630	C1D	735	C	1	19.458	41.690	2.760	1.00	14.73
2631	C1X	735	C	1	19.838	43.096	3.263	1.00	16.66
2632	C1Y	735	C	1	18.087	41.870	1.985	1.00	16.99
2633	O1E	735	C	1	20.617	41.213	1.907	1.00	15.62

2634	C1F	735	C	1	20.412	40.092	1.049	1.00	12.70
2635	C1G	735	C	1	20.433	40.315	-0.334	1.00	16.64
2636	C1I	735	C	1	20.226	39.243	-1.204	1.00	15.86
2637	C1K	735	C	1	19.985	37.892	-0.696	1.00	15.12
2638	C1J	735	C	1	19.969	37.669	0.700	1.00	15.25
2639	C1H	735	C	1	20.181	38.761	1.576	1.00	16.34
2640	C1L	735	C	1	19.744	36.701	-1.667	1.00	16.46
2641	N1M	735	C	1	19.050	37.255	-2.868	1.00	16.48
2642	C2A	735	C	1	17.700	37.386	-3.035	1.00	19.45
2643	O2A	735	C	1	16.905	37.016	-2.143	1.00	20.40
2644	S2C	735	C	1	15.441	38.082	-4.381	1.00	18.50
2645	C2B	735	C	1	17.156	37.942	-4.212	1.00	18.76
2646	C2D	735	C	1	17.793	38.466	-5.406	1.00	19.70
2647	C2G	735	C	1	19.306	38.558	-5.720	1.00	20.26
2648	N2E	735	C	1	16.928	38.919	-6.324	1.00	17.68
2649	C2F	735	C	1	15.614	38.789	-5.945	1.00	19.94
2650	C2H	735	C	1	14.528	39.186	-6.744	1.00	21.71
2651	C2J	735	C	1	13.173	39.004	-6.286	1.00	20.47
2652	C2L	735	C	1	12.084	39.400	-7.096	1.00	22.73
2653	C2M	735	C	1	12.305	39.993	-8.391	1.00	20.47
2654	C2K	735	C	1	13.651	40.175	-8.842	1.00	23.90
2655	C2I	735	C	1	14.735	39.782	-8.042	1.00	22.13
2656	C2N	735	C	1	11.115	40.435	-9.308	1.00	25.97
2657	F2P	735	C	1	10.952	39.499	-10.296	1.00	31.88
2658	F2Q	735	C	1	9.934	40.532	-8.627	1.00	31.88
2659	F2O	735	C	1	11.362	41.644	-9.892	1.00	31.88

TABLE 3

ATOMIC STRUCTURE COORDINATE DATA OBTAINED FROM X-RAY DIFFRACTION FROM THE LIGAND BINDING DOMAIN OF PPARα USED IN MOLECULAR REPLACEMENT

ATOM	ATOM TYPE	RESIDUE	PROTEIN #	#	X	Y	Z	OCC	B
1	CB	ASP	A	211	14.51	5.574	19.848	1.00	78.46
2	CG	ASP	A	211	14.259	4.095	20.068	1.00	79.53
3	OD1	ASP	A	211	13.363	3.535	19.4	1.00	80.23
4	OD2	ASP	A	211	14.961	3.492	20.908	1.00	80.14
5	C	ASP	A	211	15.241	7.375	18.272	1.00	76.33
6	O	ASP	A	211	14.371	8.176	17.929	1.00	76.50
7	N	ASP	A	211	16.106	5.066	18.029	1.00	77.36
8	CA	ASP	A	211	14.923	5.889	18.409	1.00	77.08
9	N	LEU	A	212	16.49	7.738	18.549	1.00	74.80
10	CA	LEU	A	212	16.926	9.125	18.438	1.00	72.96
11	CB	LEU	A	212	18.142	9.393	19.328	1.00	73.58
12	CG	LEU	A	212	18.809	10.76	19.098	1.00	73.64
13	CD1	LEU	A	212	18.094	11.83	19.907	1.00	73.44
14	CD2	LEU	A	212	20.274	10.68	19.492	1.00	73.65
15	C	LEU	A	212	17.315	9.398	16.997	1.00	71.55
16	O	LEU	A	212	17.304	10.54	16.548	1.00	71.54
17	N	LYS	A	213	17.672	8.346	16.274	1.00	69.51
18	CA	LYS	A	213	18.069	8.512	14.89	1.00	67.63
19	CB	LYS	A	213	18.837	7.279	14.416	1.00	68.39
20	CG	LYS	A	213	19.477	7.423	13.047	1.00	68.94
21	CD	LYS	A	213	20.908	6.9	13.051	1.00	69.41
22	CE	LYS	A	213	21.036	5.602	13.837	1.00	69.58
23	NZ	LYS	A	213	22.361	4.97	13.652	1.00	70.30
24	C	LYS	A	213	16.845	8.769	14.018	1.00	65.91
25	O	LYS	A	213	16.97	9.16	12.856	1.00	66.04
26	N	SER	A	214	15.661	8.558	14.587	1.00	62.82
27	CA	SER	A	214	14.425	8.817	13.86	1.00	59.48

28	CB	SER	A	214	13.216	8.267	14.624	1.00	59.65
29	OG	SER	A	214	12.983	9	15.815	1.00	59.47
30	C	SER	A	214	14.326	10.34	13.76	1.00	56.82
31	O	SER	A	214	13.501	10.87	13.019	1.00	56.27
32	N	LEU	A	215	15.183	11.01	14.524	1.00	53.62
33	CA	LEU	A	215	15.244	12.47	14.553	1.00	50.75
34	CB	LEU	A	215	16.368	12.93	15.49	1.00	50.59
35	CG	LEU	A	215	16.736	14.42	15.548	1.00	49.94
36	CD1	LEU	A	215	15.58	15.23	16.111	1.00	49.18
37	CD2	LEU	A	215	17.975	14.6	16.414	1.00	49.63
38	C	LEU	A	215	15.496	13.02	13.155	1.00	48.97
39	O	LEU	A	215	15.029	14.1	12.809	1.00	49.11
40	N	ALA	A	216	16.238	12.26	12.355	1.00	46.47
41	CA	ALA	A	216	16.553	12.66	10.994	1.00	45.03
42	CB	ALA	A	216	17.423	11.61	10.322	1.00	44.87
43	C	ALA	A	216	15.288	12.9	10.169	1.00	44.53
44	O	ALA	A	216	15.076	14	9.662	1.00	43.47
45	N	LYS	A	217	14.446	11.88	10.041	1.00	43.76
46	CA	LYS	A	217	13.219	12.02	9.264	1.00	42.20
47	CB	LYS	A	217	12.458	10.69	9.203	1.00	44.47
48	CG	LYS	A	217	11.537	10.58	7.988	1.00	45.43
49	CD	LYS	A	217	10.703	9.314	7.994	1.00	46.92
50	CE	LYS	A	217	9.639	9.354	9.08	1.00	48.09
51	NZ	LYS	A	217	8.771	8.147	9.043	1.00	49.24
52	C	LYS	A	217	12.325	13.09	9.866	1.00	41.19
53	O	LYS	A	217	11.653	13.83	9.145	1.00	40.18
54	N	ARG	A	218	12.325	13.18	11.193	1.00	38.94
55	CA	ARG	A	218	11.534	14.18	11.901	1.00	37.26
56	CB	ARG	A	218	11.748	14.03	13.411	1.00	39.88
57	CG	ARG	A	218	11.396	15.26	14.24	1.00	43.03
58	CD	ARG	A	218	9.903	15.54	14.26	1.00	45.71
59	NE	ARG	A	218	9.619	16.9	14.734	1.00	46.98
60	CZ	ARG	A	218	8.399	17.41	14.851	1.00	47.56
61	NH1	ARG	A	218	7.335	16.68	14.531	1.00	48.63

62	NH2	ARG	A	218	8.242	18.65	15.28	1.00	47.03
63	C	ARG	A	218	11.948	15.58	11.444	1.00	34.87
64	O	ARG	A	218	11.109	16.39	11.052	1.00	33.63
65	N	ILE	A	219	13.247	15.86	11.5	1.00	31.60
66	CA	ILE	A	219	13.762	17.16	11.084	1.00	28.45
67	CB	ILE	A	219	15.285	17.27	11.356	1.00	27.35
68	CG2	ILE	A	219	15.874	18.46	10.625	1.00	26.86
69	CG1	ILE	A	219	15.53	17.39	12.863	1.00	27.32
70	CD1	ILE	A	219	16.997	17.3	13.258	1.00	26.22
71	C	ILE	A	219	13.486	17.35	9.597	1.00	27.44
72	O	ILE	A	219	13.153	18.45	9.153	1.00	26.71
73	N	TYR	A	220	13.619	16.28	8.834	1.00	25.68
74	CA	TYR	A	220	13.374	16.33	7.402	1.00	26.73
75	CB	TYR	A	220	13.786	15.01	6.748	1.00	25.17
76	CG	TYR	A	220	13.663	14.97	5.236	1.00	27.92
77	CD1	TYR	A	220	13.856	16.12	4.465	1.00	27.10
78	CE1	TYR	A	220	13.779	16.07	3.074	1.00	27.40
79	CD2	TYR	A	220	13.391	13.77	4.572	1.00	28.20
80	CE2	TYR	A	220	13.316	13.72	3.18	1.00	29.60
81	CZ	TYR	A	220	13.512	14.88	2.438	1.00	28.67
82	OH	TYR	A	220	13.453	14.83	1.062	1.00	30.22
83	C	TYR	A	220	11.895	16.64	7.155	1.00	26.35
84	O	TYR	A	220	11.554	17.41	6.263	1.00	22.94
85	N	GLU	A	221	11.013	16.04	7.948	1.00	27.41
86	CA	GLU	A	221	9.589	16.29	7.775	1.00	27.15
87	CB	GLU	A	221	8.76	15.39	8.694	1.00	29.37
88	CG	GLU	A	221	8.871	13.92	8.317	1.00	32.72
89	CD	GLU	A	221	7.949	13.01	9.119	1.00	34.56
90	OE1	GLU	A	221	8.047	13	10.363	1.00	36.22
91	OE2	GLU	A	221	7.127	12.31	8.498	1.00	36.44
92	C	GLU	A	221	9.301	17.77	8.056	1.00	25.89
93	O	GLU	A	221	8.54	18.4	7.329	1.00	25.26
94	N	ALA	A	222	9.929	18.3	9.099	1.00	23.75
95	CA	ALA	A	222	9.749	19.7	9.463	1.00	22.66

96	CB	ALA	A	222	10.526	20.02	10.733	1.00	24.94
97	C	ALA	A	222	10.225	20.6	8.325	1.00	21.68
98	O	ALA	A	222	9.625	21.64	8.041	1.00	20.08
99	N	TYR	A	223	11.311	20.2	7.678	1.00	20.59
100	CA	TYR	A	223	11.875	20.95	6.567	1.00	20.21
101	CB	TYR	A	223	13.226	20.34	6.205	1.00	21.59
102	CG	TYR	A	223	13.893	20.85	4.95	1.00	20.23
103	CD1	TYR	A	223	13.563	20.31	3.702	1.00	21.49
104	CE1	TYR	A	223	14.255	20.69	2.557	1.00	20.65
105	CD2	TYR	A	223	14.93	21.77	5.017	1.00	19.83
106	CE2	TYR	A	223	15.631	22.15	3.874	1.00	20.40
107	CZ	TYR	A	223	15.289	21.6	2.65	1.00	20.09
108	OH	TYR	A	223	16.005	21.93	1.52	1.00	22.28
109	C	TYR	A	223	10.919	20.96	5.371	1.00	20.36
110	O	TYR	A	223	10.657	22.01	4.78	1.00	18.08
111	N	LEU	A	224	10.374	19.8	5.03	1.00	19.65
112	CA	LEU	A	224	9.455	19.72	3.901	1.00	21.64
113	CB	LEU	A	224	9.163	18.25	3.565	1.00	22.15
114	CG	LEU	A	224	10.345	17.45	3.016	1.00	23.81
115	CD1	LEU	A	224	9.94	15.99	2.85	1.00	24.83
116	CD2	LEU	A	224	10.791	18.05	1.68	1.00	24.52
117	C	LEU	A	224	8.144	20.46	4.167	1.00	21.59
118	O	LEU	A	224	7.521	20.99	3.25	1.00	22.21
119	N	LYS	A	225	7.729	20.51	5.424	1.00	21.23
120	CA	LYS	A	225	6.482	21.17	5.776	1.00	24.07
121	CB	LYS	A	225	5.972	20.61	7.11	1.00	27.04
122	CG	LYS	A	225	4.766	21.32	7.725	1.00	32.48
123	CD	LYS	A	225	5.179	22.54	8.533	1.00	34.35
124	CE	LYS	A	225	3.985	23.17	9.244	1.00	36.46
125	NZ	LYS	A	225	4.381	24.35	10.071	1.00	35.63
126	C	LYS	A	225	6.571	22.69	5.862	1.00	23.63
127	O	LYS	A	225	5.582	23.39	5.616	1.00	22.64
128	N	ASN	A	226	7.757	23.21	6.177	1.00	21.43
129	CA	ASN	A	226	7.923	24.65	6.369	1.00	21.60

130	CB	ASN	A	226	8.631	24.88	7.704	1.00	21.30
131	CG	ASN	A	226	7.739	24.56	8.883	1.00	21.85
132	OD1	ASN	A	226	6.769	25.28	9.142	1.00	21.90
133	ND2	ASN	A	226	8.046	23.48	9.592	1.00	21.00
134	C	ASN	A	226	8.576	25.51	5.305	1.00	20.24
135	O	ASN	A	226	8.481	26.74	5.373	1.00	21.01
136	N	PHE	A	227	9.229	24.9	4.326	1.00	19.71
137	CA	PHE	A	227	9.883	25.69	3.279	1.00	20.43
138	CB	PHE	A	227	11.354	25.29	3.161	1.00	19.13
139	CG	PHE	A	227	12.162	25.6	4.392	1.00	18.17
140	CD1	PHE	A	227	12.348	26.92	4.801	1.00	16.25
141	CD2	PHE	A	227	12.736	24.58	5.136	1.00	16.60
142	CE1	PHE	A	227	13.094	27.21	5.935	1.00	16.71
143	CE2	PHE	A	227	13.488	24.86	6.275	1.00	17.69
144	CZ	PHE	A	227	13.668	26.18	6.678	1.00	18.05
145	C	PHE	A	227	9.185	25.5	1.941	1.00	21.87
146	O	PHE	A	227	9.147	24.41	1.401	1.00	23.21
147	N	ASN	A	228	8.644	26.59	1.407	1.00	22.66
148	CA	ASN	A	228	7.937	26.53	0.136	1.00	23.56
149	CB	ASN	A	228	7.251	27.87	-0.135	1.00	26.95
150	CG	ASN	A	228	6.072	28.12	0.801	1.00	29.92
151	OD1	ASN	A	228	5.14	27.31	0.867	1.00	33.43
152	ND2	ASN	A	228	6.108	29.23	1.528	1.00	32.80
153	C	ASN	A	228	8.842	26.14	-1.028	1.00	23.59
154	O	ASN	A	228	8.375	25.6	-2.029	1.00	22.24
155	N	MET	A	229	10.136	26.41	-0.891	1.00	22.41
156	CA	MET	A	229	11.09	26.05	-1.931	1.00	23.18
157	CB	MET	A	229	11.724	27.31	-2.537	1.00	23.66
158	CG	MET	A	229	12.717	27.05	-3.673	1.00	25.31
159	SD	MET	A	229	11.966	26.31	-5.134	1.00	26.48
160	CE	MET	A	229	10.916	27.66	-5.681	1.00	24.83
161	C	MET	A	229	12.175	25.18	-1.328	1.00	23.23
162	O	MET	A	229	12.629	25.42	-0.206	1.00	23.23
163	N	ASN	A	230	12.56	24.14	-2.067	1.00	21.71

164	CA	ASN	A	230	13.62	23.24	-1.638	1.00	22.22
165	CB	ASN	A	230	13.057	22.03	-0.889	1.00	23.15
166	CG	ASN	A	230	12.073	21.23	-1.712	1.00	24.30
167	OD1	ASN	A	230	12.321	20.93	-2.874	1.00	25.96
168	ND2	ASN	A	230	10.952	20.87	-1.1	1.00	26.83
169	C	ASN	A	230	14.37	22.82	-2.891	1.00	22.09
170	O	ASN	A	230	13.995	23.21	-3.997	1.00	20.57
171	N	LYS	A	231	15.42	22.03	-2.728	1.00	20.59
172	CA	LYS	A	231	16.235	21.61	-3.861	1.00	20.89
173	CB	LYS	A	231	17.466	20.85	-3.364	1.00	21.48
174	CG	LYS	A	231	18.656	20.95	-4.295	1.00	20.77
175	CD	LYS	A	231	19.92	20.5	-3.597	1.00	21.19
176	CE	LYS	A	231	21.125	20.63	-4.496	1.00	21.09
177	NZ	LYS	A	231	22.355	20.17	-3.814	1.00	19.55
178	C	LYS	A	231	15.503	20.79	-4.916	1.00	20.69
179	O	LYS	A	231	15.676	21.02	-6.11	1.00	19.10
180	N	VAL	A	232	14.694	19.82	-4.494	1.00	20.29
181	CA	VAL	A	232	13.956	19.02	-5.462	1.00	23.64
182	CB	VAL	A	232	13.006	18.01	-4.772	1.00	25.30
183	CG1	VAL	A	232	12.237	17.23	-5.824	1.00	28.94
184	CG2	VAL	A	232	13.796	17.07	-3.894	1.00	28.35
185	C	VAL	A	232	13.125	19.93	-6.371	1.00	22.27
186	O	VAL	A	232	13.222	19.84	-7.596	1.00	22.87
187	N	LYS	A	233	12.32	20.8	-5.762	1.00	22.90
188	CA	LYS	A	233	11.463	21.73	-6.505	1.00	22.56
189	CB	LYS	A	233	10.644	22.6	-5.544	1.00	25.17
190	CG	LYS	A	233	9.504	21.91	-4.817	1.00	25.33
191	CD	LYS	A	233	8.687	22.94	-4.048	1.00	27.14
192	CE	LYS	A	233	7.448	22.35	-3.407	1.00	27.11
193	NZ	LYS	A	233	6.64	23.42	-2.749	1.00	25.12
194	C	LYS	A	233	12.253	22.64	-7.438	1.00	23.61
195	O	LYS	A	233	11.887	22.83	-8.603	1.00	22.28
196	N	ALA	A	234	13.331	23.22	-6.917	1.00	22.21
197	CA	ALA	A	234	14.173	24.12	-7.696	1.00	21.88

198	CB	ALA	A	234	15.239	24.74	-6.796	1.00	19.12
199	C	ALA	A	234	14.839	23.43	-8.884	1.00	22.78
200	O	ALA	A	234	14.852	23.96	-9.989	1.00	23.11
201	N	ARG	A	235	15.395	22.24	-8.665	1.00	23.76
202	CA	ARG	A	235	16.064	21.52	-9.745	1.00	26.20
203	CB	ARG	A	235	16.735	20.25	-9.208	1.00	27.83
204	CG	ARG	A	235	18.065	20.54	-8.523	1.00	28.58
205	CD	ARG	A	235	19.004	21.27	-9.478	1.00	32.23
206	NE	ARG	A	235	20.002	22.08	-8.784	1.00	34.36
207	CZ	ARG	A	235	19.701	23.04	-7.919	1.00	37.04
208	NH1	ARG	A	235	18.431	23.31	-7.639	1.00	39.09
209	NH2	ARG	A	235	20.662	23.76	-7.352	1.00	35.24
210	C	ARG	A	235	15.153	21.19	-10.92	1.00	27.67
211	O	ARG	A	235	15.6	21.18	-12.07	1.00	29.64
212	N	VAL	A	236	13.881	20.92	-10.64	1.00	27.53
213	CA	VAL	A	236	12.921	20.63	-11.7	1.00	28.83
214	CB	VAL	A	236	11.55	20.23	-11.12	1.00	30.09
215	CG1	VAL	A	236	10.493	20.23	-12.22	1.00	31.75
216	CG2	VAL	A	236	11.641	18.85	-10.49	1.00	31.01
217	C	VAL	A	236	12.734	21.88	-12.55	1.00	28.74
218	O	VAL	A	236	12.763	21.83	-13.78	1.00	27.81
219	N	ILE	A	237	12.543	23.01	-11.87	1.00	26.31
220	CA	ILE	A	237	12.346	24.28	-12.54	1.00	26.14
221	CB	ILE	A	237	12.041	25.39	-11.51	1.00	24.59
222	CG2	ILE	A	237	12.015	26.76	-12.18	1.00	23.06
223	CG1	ILE	A	237	10.7	25.1	-10.83	1.00	23.57
224	CD1	ILE	A	237	10.402	26	-9.639	1.00	25.78
225	C	ILE	A	237	13.571	24.67	-13.37	1.00	28.37
226	O	ILE	A	237	13.441	25.23	-14.46	1.00	27.38
227	N	LEU	A	238	14.756	24.34	-12.86	1.00	28.44
228	CA	LEU	A	238	16.006	24.67	-13.54	1.00	31.74
229	CB	LEU	A	238	17.133	24.78	-12.52	1.00	30.50
230	CG	LEU	A	238	17.026	25.98	-11.57	1.00	30.22
231	CD1	LEU	A	238	18.016	25.83	-10.42	1.00	29.46

232	CD2	LEU	A	238	17.283	27.26	-12.35	1.00	29.52
233	C	LEU	A	238	16.415	23.68	-14.62	1.00	34.68
234	O	LEU	A	238	17.29	23.96	-15.44	1.00	35.11
235	N	SER	A	239	15.793	22.51	-14.62	1.00	37.91
236	CA	SER	A	239	16.1	21.48	-15.6	1.00	42.67
237	CB	SER	A	239	17.408	20.77	-15.26	1.00	42.74
238	OG	SER	A	239	18.474	21.25	-16.05	1.00	44.54
239	C	SER	A	239	14.991	20.46	-15.67	1.00	45.44
240	O	SER	A	239	14.579	19.89	-14.66	1.00	46.52
241	N	GLY	A	240	14.513	20.21	-16.88	1.00	48.97
242	CA	GLY	A	240	13.452	19.25	-17.04	1.00	52.46
243	C	GLY	A	240	12.655	19.58	-18.27	1.00	55.01
244	O	GLY	A	240	12.16	18.68	-18.93	1.00	55.62
245	N	LYS	A	241	12.554	20.88	-18.57	1.00	57.05
246	CA	LYS	A	241	11.817	21.41	-19.72	1.00	58.42
247	CB	LYS	A	241	12.707	21.39	-20.96	1.00	59.37
248	CG	LYS	A	241	13.824	22.43	-20.95	1.00	58.74
249	CD	LYS	A	241	14.872	22.09	-21.99	1.00	59.57
250	CE	LYS	A	241	15.865	23.22	-22.2	1.00	59.20
251	NZ	LYS	A	241	15.485	24.06	-23.36	1.00	60.11
252	C	LYS	A	241	10.514	20.68	-20.01	1.00	59.28
253	O	LYS	A	241	9.52	21.3	-20.37	1.00	59.75
254	N	ALA	A	242	10.544	19.36	-19.85	1.00	60.20
255	CA	ALA	A	242	9.408	18.47	-20.04	1.00	60.65
256	CB	ALA	A	242	9.225	17.59	-18.81	1.00	60.60
257	C	ALA	A	242	8.152	19.27	-20.3	1.00	61.11
258	O	ALA	A	242	7.718	19.43	-21.44	1.00	61.12
259	N	SER	A	243	7.581	19.79	-19.21	1.00	61.07
260	CA	SER	A	243	6.382	20.59	-19.3	1.00	61.06
261	CB	SER	A	243	5.726	20.72	-17.92	1.00	61.00
262	OG	SER	A	243	4.64	21.63	-17.95	1.00	59.89
263	C	SER	A	243	6.742	21.98	-19.84	1.00	61.10
264	O	SER	A	243	7.434	22.11	-20.85	1.00	61.74
265	N	ASN	A	244	6.279	23.01	-19.14	1.00	60.20

266	CA	ASN	A	244	6.53	24.38	-19.55	1.00	59.10
267	CB	ASN	A	244	5.91	24.6	-20.95	1.00	58.65
268	CG	ASN	A	244	5.63	26.05	-21.26	1.00	58.90
269	OD1	ASN	A	244	4.647	26.62	-20.78	1.00	59.73
270	ND2	ASN	A	244	6.488	26.66	-22.07	1.00	58.39
271	C	ASN	A	244	5.964	25.34	-18.5	1.00	58.52
272	O	ASN	A	244	5.616	24.91	-17.4	1.00	59.67
273	N	ASN	A	245	5.873	26.62	-18.85	1.00	56.14
274	CA	ASN	A	245	5.406	27.68	-17.94	1.00	51.26
275	CB	ASN	A	245	4.324	27.13	-17.01	1.00	52.89
276	CG	ASN	A	245	4.047	28.05	-15.84	1.00	52.48
277	OD1	ASN	A	245	3.453	29.12	-16	1.00	52.78
278	ND2	ASN	A	245	4.489	27.64	-14.66	1.00	52.90
279	C	ASN	A	245	6.685	28.03	-17.18	1.00	47.02
280	O	ASN	A	245	6.689	28.2	-15.96	1.00	47.14
281	N	PRO	A	246	7.789	28.19	-17.93	1.00	42.04
282	CD	PRO	A	246	7.619	28.47	-19.37	1.00	41.47
283	CA	PRO	A	246	9.161	28.51	-17.54	1.00	38.16
284	CB	PRO	A	246	9.88	28.58	-18.87	1.00	38.68
285	CG	PRO	A	246	8.86	29.26	-19.71	1.00	39.97
286	C	PRO	A	246	9.379	29.77	-16.74	1.00	34.87
287	O	PRO	A	246	8.668	30.76	-16.9	1.00	34.21
288	N	PRO	A	247	10.379	29.75	-15.85	1.00	32.12
289	CD	PRO	A	247	11.207	28.6	-15.43	1.00	32.31
290	CA	PRO	A	247	10.669	30.93	-15.04	1.00	29.30
291	CB	PRO	A	247	11.823	30.47	-14.14	1.00	29.79
292	CG	PRO	A	247	12.418	29.28	-14.88	1.00	32.45
293	C	PRO	A	247	11.053	32.07	-15.97	1.00	27.36
294	O	PRO	A	247	11.692	31.86	-17.01	1.00	25.06
295	N	PHE	A	248	10.639	33.28	-15.62	1.00	24.30
296	CA	PHE	A	248	10.943	34.45	-16.43	1.00	23.14
297	CB	PHE	A	248	10.004	35.6	-16.07	1.00	25.05
298	CG	PHE	A	248	10.098	36.76	-17.01	1.00	26.31
299	CD1	PHE	A	248	9.46	36.72	-18.25	1.00	27.99

300	CD2	PHE	A	248	10.865	37.87	-16.69	1.00	27.41
301	CE1	PHE	A	248	9.585	37.77	-19.15	1.00	28.47
302	CE2	PHE	A	248	10.999	38.93	-17.59	1.00	28.03
303	CZ	PHE	A	248	10.357	38.88	-18.82	1.00	29.16
304	C	PHE	A	248	12.371	34.87	-16.13	1.00	22.55
305	O	PHE	A	248	12.726	35.08	-14.98	1.00	19.83
306	N	VAL	A	249	13.188	35	-17.17	1.00	22.23
307	CA	VAL	A	249	14.578	35.38	-16.97	1.00	21.89
308	CB	VAL	A	249	15.49	34.73	-18.04	1.00	23.08
309	CG1	VAL	A	249	16.917	35.26	-17.91	1.00	22.71
310	CG2	VAL	A	249	15.484	33.21	-17.87	1.00	22.78
311	C	VAL	A	249	14.817	36.88	-16.96	1.00	22.84
312	O	VAL	A	249	14.41	37.61	-17.87	1.00	22.43
313	N	ILE	A	250	15.472	37.34	-15.89	1.00	20.77
314	CA	ILE	A	250	15.814	38.74	-15.73	1.00	20.91
315	CB	ILE	A	250	15.494	39.22	-14.3	1.00	20.98
316	CG2	ILE	A	250	15.899	40.69	-14.14	1.00	19.06
317	CG1	ILE	A	250	13.996	39.04	-14.02	1.00	19.24
318	CD1	ILE	A	250	13.602	39.29	-12.57	1.00	21.68
319	C	ILE	A	250	17.314	38.83	-16	1.00	21.63
320	O	ILE	A	250	18.134	38.4	-15.18	1.00	19.53
321	N	HIS	A	251	17.668	39.37	-17.17	1.00	20.99
322	CA	HIS	A	251	19.07	39.48	-17.56	1.00	22.26
323	CB	HIS	A	251	19.343	38.57	-18.76	1.00	24.28
324	CG	HIS	A	251	18.57	38.93	-19.99	1.00	24.97
325	CD2	HIS	A	251	17.449	38.4	-20.53	1.00	25.77
326	ND1	HIS	A	251	18.922	39.99	-20.8	1.00	27.65
327	CE1	HIS	A	251	18.049	40.09	-21.79	1.00	25.99
328	NE2	HIS	A	251	17.145	39.14	-21.65	1.00	26.18
329	C	HIS	A	251	19.535	40.9	-17.86	1.00	23.10
330	O	HIS	A	251	20.719	41.13	-18.11	1.00	21.51
331	N	ASP	A	252	18.601	41.85	-17.84	1.00	23.64
332	CA	ASP	A	252	18.912	43.26	-18.07	1.00	26.61
333	CB	ASP	A	252	19.179	43.55	-19.55	1.00	27.87

334	CG	ASP	A	252	17.985	43.26	-20.44	1.00	29.61
335	OD1	ASP	A	252	16.857	43.13	-19.92	1.00	28.47
336	OD2	ASP	A	252	18.181	43.18	-21.68	1.00	31.76
337	C	ASP	A	252	17.791	44.15	-17.55	1.00	27.23
338	O	ASP	A	252	16.797	43.67	-17.01	1.00	25.64
339	N	MET	A	253	17.951	45.46	-17.73	1.00	28.20
340	CA	MET	A	253	16.958	46.41	-17.25	1.00	28.88
341	CB	MET	A	253	17.459	47.83	-17.49	1.00	31.16
342	CG	MET	A	253	18.755	48.11	-16.76	1.00	33.46
343	SD	MET	A	253	18.548	48.1	-14.96	1.00	36.77
344	CE	MET	A	253	19.322	49.69	-14.59	1.00	37.18
345	C	MET	A	253	15.566	46.24	-17.84	1.00	28.34
346	O	MET	A	253	14.565	46.4	-17.14	1.00	27.10
347	N	GLU	A	254	15.493	45.89	-19.12	1.00	28.20
348	CA	GLU	A	254	14.199	45.71	-19.76	1.00	27.38
349	CB	GLU	A	254	14.368	45.54	-21.28	1.00	30.74
350	CG	GLU	A	254	13.066	45.25	-22	1.00	34.46
351	CD	GLU	A	254	13.222	45.23	-23.51	1.00	37.18
352	OE1	GLU	A	254	14.097	44.5	-24.02	1.00	38.99
353	OE2	GLU	A	254	12.46	45.95	-24.19	1.00	39.82
354	C	GLU	A	254	13.443	44.51	-19.19	1.00	26.77
355	O	GLU	A	254	12.267	44.62	-18.84	1.00	24.55
356	N	THR	A	255	14.116	43.37	-19.09	1.00	25.14
357	CA	THR	A	255	13.476	42.17	-18.55	1.00	22.92
358	CB	THR	A	255	14.335	40.91	-18.81	1.00	22.22
359	OG1	THR	A	255	15.677	41.13	-18.36	1.00	20.92
360	CG2	THR	A	255	14.349	40.58	-20.3	1.00	22.08
361	C	THR	A	255	13.167	42.3	-17.06	1.00	22.64
362	O	THR	A	255	12.277	41.62	-16.54	1.00	21.75
363	N	LEU	A	256	13.895	43.17	-16.36	1.00	21.77
364	CA	LEU	A	256	13.629	43.39	-14.94	1.00	20.25
365	CB	LEU	A	256	14.7	44.28	-14.29	1.00	20.20
366	CG	LEU	A	256	14.347	44.72	-12.86	1.00	18.26
367	CD1	LEU	A	256	14.292	43.5	-11.94	1.00	19.55

368	CD2	LEU	A	256	15.378	45.72	-12.34	1.00	17.68
369	C	LEU	A	256	12.282	44.09	-14.84	1.00	20.44
370	O	LEU	A	256	11.424	43.7	-14.06	1.00	19.24
371	N	CYS	A	257	12.092	45.13	-15.64	1.00	20.05
372	CA	CYS	A	257	10.828	45.85	-15.61	1.00	22.13
373	CB	CYS	A	257	10.893	47.09	-16.53	1.00	22.88
374	SG	CYS	A	257	12.084	48.36	-16	1.00	28.89
375	C	CYS	A	257	9.675	44.94	-16.02	1.00	22.46
376	O	CYS	A	257	8.588	45.02	-15.46	1.00	23.21
377	N	MET	A	258	9.915	44.06	-17	1.00	24.21
378	CA	MET	A	258	8.881	43.13	-17.47	1.00	25.70
379	CB	MET	A	258	9.383	42.33	-18.67	1.00	28.67
380	CG	MET	A	258	9.875	43.17	-19.85	1.00	34.04
381	SD	MET	A	258	10.485	42.19	-21.26	1.00	38.98
382	CE	MET	A	258	10.123	43.33	-22.62	1.00	38.27
383	C	MET	A	258	8.496	42.18	-16.34	1.00	25.87
384	O	MET	A	258	7.314	41.92	-16.1	1.00	25.43
385	N	ALA	A	259	9.503	41.64	-15.66	1.00	24.88
386	CA	ALA	A	259	9.262	40.72	-14.56	1.00	23.76
387	CB	ALA	A	259	10.586	40.19	-14.03	1.00	22.98
388	C	ALA	A	259	8.482	41.41	-13.44	1.00	22.99
389	O	ALA	A	259	7.546	40.83	-12.89	1.00	23.42
390	N	GLU	A	260	8.864	42.64	-13.12	1.00	22.90
391	CA	GLU	A	260	8.178	43.38	-12.07	1.00	23.30
392	CB	GLU	A	260	8.843	44.75	-11.85	1.00	23.04
393	CG	GLU	A	260	10.269	44.67	-11.31	1.00	23.77
394	CD	GLU	A	260	10.974	46.02	-11.26	1.00	25.32
395	OE1	GLU	A	260	10.929	46.75	-12.27	1.00	26.09
396	OE2	GLU	A	260	11.59	46.34	-10.23	1.00	24.65
397	C	GLU	A	260	6.717	43.57	-12.46	1.00	24.60
398	O	GLU	A	260	5.818	43.41	-11.64	1.00	23.99
399	N	LYS	A	261	6.489	43.91	-13.72	1.00	26.88
400	CA	LYS	A	261	5.138	44.13	-14.22	1.00	29.38
401	CB	LYS	A	261	5.18	44.42	-15.72	1.00	31.11

402	CG	LYS	A	261	3.818	44.72	-16.31	1.00	34.55
403	CD	LYS	A	261	3.758	46.12	-16.89	1.00	38.59
404	CE	LYS	A	261	4.149	47.18	-15.87	1.00	40.59
405	NZ	LYS	A	261	5.627	47.33	-15.75	1.00	42.89
406	C	LYS	A	261	4.233	42.92	-13.96	1.00	30.43
407	O	LYS	A	261	3.05	43.07	-13.65	1.00	30.61
408	N	THR	A	262	4.797	41.72	-14.08	1.00	31.64
409	CA	THR	A	262	4.031	40.5	-13.88	1.00	32.66
410	CB	THR	A	262	4.501	39.39	-14.85	1.00	34.32
411	OG1	THR	A	262	4.522	39.9	-16.19	1.00	37.49
412	CG2	THR	A	262	3.551	38.2	-14.79	1.00	34.76
413	C	THR	A	262	4.078	39.92	-12.47	1.00	32.57
414	O	THR	A	262	3.04	39.59	-11.89	1.00	33.27
415	N	LEU	A	263	5.279	39.8	-11.91	1.00	31.54
416	CA	LEU	A	263	5.453	39.21	-10.58	1.00	31.84
417	CB	LEU	A	263	6.819	38.53	-10.51	1.00	32.07
418	CG	LEU	A	263	6.945	37.14	-11.14	1.00	33.07
419	CD1	LEU	A	263	5.767	36.84	-12.06	1.00	32.88
420	CD2	LEU	A	263	8.261	37.06	-11.88	1.00	32.53
421	C	LEU	A	263	5.275	40.13	-9.371	1.00	32.52
422	O	LEU	A	263	4.808	39.68	-8.319	1.00	31.50
423	N	VAL	A	264	5.662	41.39	-9.504	1.00	32.08
424	CA	VAL	A	264	5.532	42.35	-8.412	1.00	32.49
425	CB	VAL	A	264	6.897	42.61	-7.727	1.00	32.30
426	CG1	VAL	A	264	6.752	43.68	-6.667	1.00	33.97
427	CG2	VAL	A	264	7.403	41.32	-7.079	1.00	33.63
428	C	VAL	A	264	4.992	43.64	-9.009	1.00	33.56
429	O	VAL	A	264	5.659	44.68	-9.012	1.00	32.17
430	N	ALA	A	265	3.768	43.55	-9.518	1.00	34.97
431	CA	ALA	A	265	3.079	44.66	-10.17	1.00	35.76
432	CB	ALA	A	265	1.623	44.28	-10.4	1.00	37.47
433	C	ALA	A	265	3.148	46.04	-9.512	1.00	37.14
434	O	ALA	A	265	3.094	47.06	-10.21	1.00	35.98
435	N	LYS	A	266	3.271	46.1	-8.189	1.00	37.87

436	CA	LYS	A	266	3.313	47.39	-7.507	1.00	39.85
437	CB	LYS	A	266	3.159	47.21	-5.989	1.00	39.30
438	CG	LYS	A	266	3.099	48.54	-5.222	1.00	40.41
439	CD	LYS	A	266	3.065	48.35	-3.709	1.00	41.21
440	CE	LYS	A	266	1.695	47.91	-3.21	1.00	42.93
441	NZ	LYS	A	266	0.646	48.94	-3.476	1.00	44.25
442	C	LYS	A	266	4.565	48.24	-7.782	1.00	40.87
443	O	LYS	A	266	4.519	49.46	-7.702	1.00	41.16
444	N	LEU	A	267	5.675	47.58	-8.11	1.00	41.92
445	CA	LEU	A	267	6.922	48.3	-8.358	1.00	43.90
446	CB	LEU	A	267	8.114	47.38	-8.094	1.00	43.36
447	CG	LEU	A	267	8.078	46.63	-6.758	1.00	42.94
448	CD1	LEU	A	267	9.45	46.03	-6.48	1.00	42.92
449	CD2	LEU	A	267	7.673	47.57	-5.63	1.00	43.54
450	C	LEU	A	267	7.054	48.92	-9.748	1.00	45.44
451	O	LEU	A	267	8.128	49.41	-10.12	1.00	45.30
452	N	VAL	A	268	5.967	48.92	-10.51	1.00	47.08
453	CA	VAL	A	268	5.986	49.49	-11.85	1.00	49.10
454	CB	VAL	A	268	5.831	48.4	-12.93	1.00	49.12
455	CG1	VAL	A	268	7.032	47.47	-12.91	1.00	49.41
456	CG2	VAL	A	268	4.547	47.62	-12.69	1.00	49.20
457	C	VAL	A	268	4.876	50.52	-12.07	1.00	50.30
458	O	VAL	A	268	4.885	51.25	-13.06	1.00	50.13
459	N	ALA	A	269	3.929	50.57	-11.13	1.00	51.85
460	CA	ALA	A	269	2.799	51.49	-11.25	1.00	53.91
461	CB	ALA	A	269	1.491	50.71	-11.16	1.00	53.84
462	C	ALA	A	269	2.779	52.65	-10.26	1.00	55.04
463	O	ALA	A	269	1.788	53.37	-10.16	1.00	55.68
464	N	GLY	A	270	3.863	52.82	-9.508	1.00	55.70
465	CA	GLY	A	270	3.921	53.9	-8.54	1.00	57.57
466	C	GLY	A	270	5.338	54.41	-8.407	1.00	58.36
467	O	GLY	A	270	5.581	55.62	-8.394	1.00	58.74
468	N	ILE	A	271	6.272	53.47	-8.31	1.00	58.34
469	CA	ILE	A	271	7.695	53.76	-8.188	1.00	57.76

470	CB	ILE	A	271	8.424	52.63	-7.416	1.00	58.40
471	CG2	ILE	A	271	9.919	52.65	-7.72	1.00	58.51
472	CG1	ILE	A	271	8.159	52.76	-5.916	1.00	58.87
473	CD1	ILE	A	271	8.831	51.68	-5.081	1.00	59.43
474	C	ILE	A	271	8.307	53.86	-9.58	1.00	57.27
475	O	ILE	A	271	8.638	54.95	-10.06	1.00	57.93
476	N	GLN	A	272	8.435	52.7	-10.21	1.00	55.75
477	CA	GLN	A	272	9.007	52.52	-11.54	1.00	54.43
478	CB	GLN	A	272	7.969	52.82	-12.64	1.00	54.62
479	CG	GLN	A	272	7.554	54.26	-12.78	1.00	54.62
480	CD	GLN	A	272	6.052	54.43	-12.71	1.00	54.37
481	OE1	GLN	A	272	5.471	54.46	-11.63	1.00	54.65
482	NE2	GLN	A	272	5.411	54.52	-13.87	1.00	53.99
483	C	GLN	A	272	10.318	53.24	-11.84	1.00	53.23
484	O	GLN	A	272	11.049	52.83	-12.74	1.00	53.33
485	N	ASN	A	274	10.634	54.31	-11.11	1.00	51.79
486	CA	ASN	A	274	11.922	54.94	-11.37	1.00	50.16
487	CB	ASN	A	274	11.843	56.1	-12.34	1.00	52.29
488	CG	ASN	A	274	13.008	56.09	-13.33	1.00	54.63
489	OD1	ASN	A	274	13.481	57.13	-13.78	1.00	56.51
490	ND2	ASN	A	274	13.472	54.89	-13.67	1.00	55.84
491	C	ASN	A	274	12.762	55.35	-10.18	1.00	47.37
492	O	ASN	A	274	13.387	56.41	-10.18	1.00	47.22
493	N	LYS	A	275	12.732	54.52	-9.146	1.00	43.69
494	CA	LYS	A	275	13.627	54.71	-8.026	1.00	38.70
495	CB	LYS	A	275	13.13	53.98	-6.779	1.00	39.95
496	CG	LYS	A	275	11.997	54.69	-6.051	1.00	41.04
497	CD	LYS	A	275	11.744	54.06	-4.686	1.00	42.78
498	CE	LYS	A	275	10.677	54.82	-3.905	1.00	43.67
499	NZ	LYS	A	275	10.448	54.23	-2.551	1.00	44.37
500	C	LYS	A	275	14.632	53.86	-8.794	1.00	35.85
501	O	LYS	A	275	14.203	53.01	-9.578	1.00	32.72
502	N	GLU	A	276	15.934	54.07	-8.645	1.00	33.11
503	CA	GLU	A	276	16.802	53.24	-9.467	1.00	30.98

504	CB	GLU	A	276	18.279	53.64	-9.331	1.00	34.18
505	CG	GLU	A	276	18.874	53.68	-7.955	1.00	36.39
506	CD	GLU	A	276	20.194	54.43	-7.958	1.00	36.02
507	OE1	GLU	A	276	21.05	54.15	-8.823	1.00	36.54
508	OE2	GLU	A	276	20.376	55.31	-7.097	1.00	38.61
509	C	GLU	A	276	16.587	51.76	-9.234	1.00	29.49
510	O	GLU	A	276	16.175	51.32	-8.157	1.00	26.80
511	N	VAL	A	277	16.834	50.98	-10.28	1.00	26.80
512	CA	VAL	A	277	16.636	49.55	-10.23	1.00	27.28
513	CB	VAL	A	277	17.141	48.89	-11.52	1.00	26.70
514	CG1	VAL	A	277	16.422	49.49	-12.71	1.00	31.18
515	CG2	VAL	A	277	18.627	49.07	-11.64	1.00	31.22
516	C	VAL	A	277	17.268	48.84	-9.038	1.00	24.93
517	O	VAL	A	277	16.65	47.95	-8.457	1.00	23.64
518	N	GLU	A	278	18.487	49.23	-8.662	1.00	22.59
519	CA	GLU	A	278	19.126	48.56	-7.539	1.00	22.23
520	CB	GLU	A	278	20.549	49.1	-7.281	1.00	23.67
521	CG	GLU	A	278	20.912	50.44	-7.901	1.00	27.55
522	CD	GLU	A	278	21.043	50.38	-9.41	1.00	24.59
523	OE1	GLU	A	278	20.075	50.75	-10.08	1.00	26.10
524	OE2	GLU	A	278	22.104	49.96	-9.927	1.00	26.97
525	C	GLU	A	278	18.3	48.65	-6.26	1.00	22.57
526	O	GLU	A	278	18.329	47.74	-5.441	1.00	21.72
527	N	VAL	A	279	17.551	49.74	-6.094	1.00	21.59
528	CA	VAL	A	279	16.731	49.9	-4.895	1.00	21.26
529	CB	VAL	A	279	16.303	51.37	-4.721	1.00	23.06
530	CG1	VAL	A	279	15.292	51.5	-3.596	1.00	25.08
531	CG2	VAL	A	279	17.53	52.22	-4.415	1.00	25.52
532	C	VAL	A	279	15.5	49	-4.947	1.00	19.49
533	O	VAL	A	279	15.058	48.47	-3.918	1.00	18.78
534	N	ARG	A	280	14.956	48.81	-6.146	1.00	18.65
535	CA	ARG	A	280	13.796	47.94	-6.338	1.00	17.90
536	CB	ARG	A	280	13.243	48.1	-7.762	1.00	18.81
537	CG	ARG	A	280	12.211	49.2	-7.895	1.00	23.01

538	CD	ARG	A	280	12.321	49.93	-9.216	1.00	23.63
539	NE	ARG	A	280	12.387	49.04	-10.37	1.00	21.82
540	CZ	ARG	A	280	12.895	49.4	-11.55	1.00	23.69
541	NH1	ARG	A	280	13.376	50.63	-11.7	1.00	25.06
542	NH2	ARG	A	280	12.928	48.55	-12.56	1.00	24.09
543	C	ARG	A	280	14.217	46.49	-6.096	1.00	17.66
544	O	ARG	A	280	13.531	45.74	-5.405	1.00	16.97
545	N	ILE	A	281	15.356	46.11	-6.661	1.00	17.24
546	CA	ILE	A	281	15.877	44.76	-6.496	1.00	16.58
547	CB	ILE	A	281	17.152	44.55	-7.34	1.00	17.41
548	CG2	ILE	A	281	17.846	43.24	-6.943	1.00	17.49
549	CG1	ILE	A	281	16.779	44.56	-8.828	1.00	17.66
550	CD1	ILE	A	281	17.964	44.53	-9.781	1.00	19.17
551	C	ILE	A	281	16.192	44.5	-5.024	1.00	16.90
552	O	ILE	A	281	15.898	43.43	-4.497	1.00	16.85
553	N	PHE	A	282	16.776	45.5	-4.359	1.00	14.57
554	CA	PHE	A	282	17.111	45.36	-2.942	1.00	13.82
555	CB	PHE	A	282	17.886	46.59	-2.455	1.00	14.33
556	CG	PHE	A	282	18.48	46.42	-1.084	1.00	16.86
557	CD1	PHE	A	282	19.595	45.62	-0.894	1.00	17.16
558	CD2	PHE	A	282	17.927	47.07	0.014	1.00	16.21
559	CE1	PHE	A	282	20.157	45.46	0.364	1.00	18.94
560	CE2	PHE	A	282	18.481	46.92	1.28	1.00	19.15
561	CZ	PHE	A	282	19.601	46.11	1.456	1.00	20.18
562	C	PHE	A	282	15.848	45.21	-2.099	1.00	14.30
563	O	PHE	A	282	15.861	44.52	-1.085	1.00	15.47
564	N	HIS	A	283	14.766	45.87	-2.498	1.00	14.52
565	CA	HIS	A	283	13.517	45.76	-1.761	1.00	15.32
566	CB	HIS	A	283	12.454	46.7	-2.334	1.00	16.74
567	CG	HIS	A	283	11.139	46.6	-1.628	1.00	18.93
568	CD2	HIS	A	283	9.966	46.04	-1.999	1.00	21.47
569	ND1	HIS	A	283	10.95	47.07	-0.345	1.00	19.40
570	CE1	HIS	A	283	9.718	46.8	0.045	1.00	21.96
571	NE2	HIS	A	283	9.1	46.17	-0.94	1.00	23.33

572	C	HIS	A	283	13.03	44.31	-1.877	1.00	14.53
573	O	HIS	A	283	12.606	43.71	-0.9	1.00	15.83
574	N	CYS	A	284	13.089	43.77	-3.086	1.00	14.60
575	CA	CYS	A	284	12.668	42.39	-3.317	1.00	14.94
576	CB	CYS	A	284	12.713	42.06	-4.81	1.00	14.09
577	SG	CYS	A	284	11.464	42.95	-5.76	1.00	16.01
578	C	CYS	A	284	13.555	41.41	-2.539	1.00	14.97
579	O	CYS	A	284	13.09	40.37	-2.088	1.00	13.78
580	N	CYS	A	285	14.835	41.75	-2.385	1.00	15.23
581	CA	CYS	A	285	15.741	40.88	-1.626	1.00	13.47
582	CB	CYS	A	285	17.179	41.42	-1.666	1.00	15.89
583	SG	CYS	A	285	17.998	41.25	-3.256	1.00	15.55
584	C	CYS	A	285	15.266	40.84	-0.179	1.00	15.09
585	O	CYS	A	285	15.27	39.79	0.466	1.00	15.43
586	N	GLN	A	286	14.857	42	0.327	1.00	13.05
587	CA	GLN	A	286	14.375	42.1	1.7	1.00	14.74
588	CB	GLN	A	286	14.151	43.56	2.098	1.00	16.57
589	CG	GLN	A	286	15.42	44.38	2.198	1.00	18.11
590	CD	GLN	A	286	15.234	45.59	3.08	1.00	20.26
591	OE1	GLN	A	286	14.974	45.47	4.278	1.00	22.83
592	NE2	GLN	A	286	15.362	46.78	2.494	1.00	22.10
593	C	GLN	A	286	13.079	41.34	1.904	1.00	14.38
594	O	GLN	A	286	12.896	40.67	2.925	1.00	14.08
595	N	CYS	A	287	12.169	41.45	0.943	1.00	14.67
596	CA	CYS	A	287	10.905	40.74	1.063	1.00	15.04
597	CB	CYS	A	287	9.982	41.09	-0.104	1.00	16.30
598	SG	CYS	A	287	9.397	42.8	-0.06	1.00	22.25
599	C	CYS	A	287	11.187	39.24	1.091	1.00	14.70
600	O	CYS	A	287	10.587	38.5	1.864	1.00	14.34
601	N	THR	A	288	12.117	38.81	0.245	1.00	14.73
602	CA	THR	A	288	12.511	37.41	0.164	1.00	14.32
603	CB	THR	A	288	13.5	37.2	-1.003	1.00	15.37
604	OG1	THR	A	288	12.863	37.59	-2.233	1.00	13.87
605	CG2	THR	A	288	13.93	35.74	-1.1	1.00	14.11

606	C	THR	A	288	13.132	36.94	1.485	1.00	14.08
607	O	THR	A	288	12.771	35.89	2.023	1.00	13.41
608	N	SER	A	289	14.05	37.73	2.03	1.00	12.61
609	CA	SER	A	289	14.664	37.37	3.305	1.00	12.61
610	CB	SER	A	289	15.769	38.36	3.659	1.00	12.19
611	OG	SER	A	289	16.916	38.11	2.875	1.00	11.40
612	C	SER	A	289	13.652	37.31	4.453	1.00	12.67
613	O	SER	A	289	13.72	36.42	5.289	1.00	12.90
614	N	VAL	A	290	12.71	38.25	4.493	1.00	13.57
615	CA	VAL	A	290	11.712	38.25	5.564	1.00	13.84
616	CB	VAL	A	290	10.78	39.48	5.455	1.00	15.55
617	CG1	VAL	A	290	9.541	39.31	6.333	1.00	17.55
618	CG2	VAL	A	290	11.549	40.72	5.887	1.00	16.53
619	C	VAL	A	290	10.905	36.96	5.536	1.00	15.35
620	O	VAL	A	290	10.64	36.35	6.578	1.00	14.98
621	N	GLU	A	291	10.536	36.52	4.338	1.00	16.73
622	CA	GLU	A	291	9.771	35.28	4.185	1.00	16.47
623	CB	GLU	A	291	9.329	35.11	2.729	1.00	19.03
624	CG	GLU	A	291	8.339	36.16	2.244	1.00	22.45
625	CD	GLU	A	291	6.917	35.91	2.726	1.00	27.72
626	OE1	GLU	A	291	6.712	35	3.567	1.00	28.03
627	OE2	GLU	A	291	6.003	36.62	2.261	1.00	27.23
628	C	GLU	A	291	10.604	34.08	4.61	1.00	15.29
629	O	GLU	A	291	10.107	33.19	5.286	1.00	14.93
630	N	THR	A	292	11.877	34.07	4.228	1.00	13.72
631	CA	THR	A	292	12.731	32.94	4.584	1.00	13.42
632	CB	THR	A	292	14.074	33.01	3.839	1.00	13.57
633	OG1	THR	A	292	13.825	33.11	2.428	1.00	13.65
634	CG2	THR	A	292	14.885	31.74	4.092	1.00	13.97
635	C	THR	A	292	12.966	32.88	6.091	1.00	13.92
636	O	THR	A	292	12.963	31.8	6.68	1.00	15.10
637	N	VAL	A	293	13.16	34.04	6.718	1.00	14.12
638	CA	VAL	A	293	13.357	34.07	8.172	1.00	14.58
639	CB	VAL	A	293	13.612	35.5	8.676	1.00	14.45

640	CG1	VAL	A	293	13.488	35.55	10.201	1.00	15.36
641	CG2	VAL	A	293	14.986	35.97	8.243	1.00	15.78
642	C	VAL	A	293	12.095	33.54	8.855	1.00	14.26
643	O	VAL	A	293	12.164	32.82	9.866	1.00	14.04
644	N	THR	A	294	10.941	33.9	8.304	1.00	15.03
645	CA	THR	A	294	9.667	33.45	8.859	1.00	16.55
646	CB	THR	A	294	8.491	34.13	8.119	1.00	17.70
647	OG1	THR	A	294	8.624	35.56	8.228	1.00	18.26
648	CG2	THR	A	294	7.154	33.71	8.721	1.00	18.59
649	C	THR	A	294	9.553	31.93	8.779	1.00	16.67
650	O	THR	A	294	9.122	31.28	9.731	1.00	15.85
651	N	GLU	A	295	9.953	31.35	7.65	1.00	16.45
652	CA	GLU	A	295	9.896	29.89	7.495	1.00	14.59
653	CB	GLU	A	295	10.204	29.48	6.047	1.00	17.05
654	CG	GLU	A	295	9.207	29.97	5.031	1.00	19.53
655	CD	GLU	A	295	9.556	29.51	3.623	1.00	21.27
656	OE1	GLU	A	295	10.759	29.44	3.297	1.00	24.29
657	OE2	GLU	A	295	8.628	29.24	2.845	1.00	26.60
658	C	GLU	A	295	10.892	29.18	8.419	1.00	15.53
659	O	GLU	A	295	10.591	28.13	8.986	1.00	14.95
660	N	LEU	A	296	12.084	29.76	8.554	1.00	14.15
661	CA	LEU	A	296	13.121	29.18	9.402	1.00	14.54
662	CB	LEU	A	296	14.421	29.98	9.243	1.00	13.35
663	CG	LEU	A	296	15.288	29.53	8.06	1.00	13.79
664	CD1	LEU	A	296	16.282	30.62	7.666	1.00	14.77
665	CD2	LEU	A	296	16.026	28.25	8.448	1.00	15.41
666	C	LEU	A	296	12.687	29.18	10.863	1.00	15.65
667	O	LEU	A	296	13.026	28.28	11.629	1.00	15.76
668	N	THR	A	297	11.942	30.21	11.241	1.00	16.74
669	CA	THR	A	297	11.467	30.33	12.613	1.00	17.31
670	CB	THR	A	297	10.823	31.72	12.827	1.00	17.24
671	OG1	THR	A	297	11.84	32.72	12.696	1.00	18.00
672	CG2	THR	A	297	10.184	31.83	14.216	1.00	18.26
673	C	THR	A	297	10.48	29.2	12.91	1.00	18.94

674	O	THR	A	297	10.518	28.61	13.99	1.00	18.36
675	N	GLU	A	298	9.61	28.9	11.947	1.00	18.64
676	CA	GLU	A	298	8.647	27.82	12.123	1.00	19.64
677	CB	GLU	A	298	7.585	27.87	11.023	1.00	20.78
678	CG	GLU	A	298	6.701	29.09	11.109	1.00	24.51
679	CD	GLU	A	298	5.986	29.17	12.439	1.00	27.16
680	OE1	GLU	A	298	5.16	28.28	12.715	1.00	28.65
681	OE2	GLU	A	298	6.256	30.12	13.208	1.00	29.29
682	C	GLU	A	298	9.375	26.48	12.099	1.00	19.12
683	O	GLU	A	298	9.006	25.55	12.817	1.00	19.43
684	N	PHE	A	299	10.403	26.38	11.258	1.00	18.63
685	CA	PHE	A	299	11.205	25.15	11.174	1.00	18.56
686	CB	PHE	A	299	12.284	25.3	10.094	1.00	18.22
687	CG	PHE	A	299	13.287	24.17	10.078	1.00	16.52
688	CD1	PHE	A	299	12.909	22.89	9.711	1.00	15.73
689	CD2	PHE	A	299	14.622	24.41	10.407	1.00	16.62
690	CE1	PHE	A	299	13.842	21.85	9.667	1.00	16.62
691	CE2	PHE	A	299	15.56	23.39	10.367	1.00	16.63
692	CZ	PHE	A	299	15.168	22.1	9.992	1.00	16.10
693	C	PHE	A	299	11.887	24.9	12.52	1.00	19.02
694	O	PHE	A	299	11.855	23.78	13.041	1.00	19.20
695	N	ALA	A	300	12.519	25.93	13.068	1.00	19.85
696	CA	ALA	A	300	13.218	25.8	14.348	1.00	19.89
697	CB	ALA	A	300	13.855	27.13	14.739	1.00	20.05
698	C	ALA	A	300	12.267	25.34	15.448	1.00	21.19
699	O	ALA	A	300	12.627	24.5	16.284	1.00	19.62
700	N	LYS	A	301	11.059	25.89	15.447	1.00	21.75
701	CA	LYS	A	301	10.052	25.54	16.444	1.00	23.62
702	CB	LYS	A	301	8.8	26.4	16.253	1.00	22.82
703	CG	LYS	A	301	8.959	27.85	16.717	1.00	27.26
704	CD	LYS	A	301	7.814	28.74	16.225	1.00	30.13
705	CE	LYS	A	301	6.447	28.16	16.557	1.00	32.35
706	NZ	LYS	A	301	6.238	27.99	18.021	1.00	36.87
707	C	LYS	A	301	9.685	24.07	16.352	1.00	24.64

708	O	LYS	A	301	9.158	23.49	17.304	1.00	24.87
709	N	ALA	A	302	9.973	23.46	15.204	1.00	24.73
710	CA	ALA	A	302	9.674	22.05	14.987	1.00	24.93
711	CB	ALA	A	302	9.181	21.84	13.563	1.00	24.81
712	C	ALA	A	302	10.864	21.13	15.277	1.00	24.71
713	O	ALA	A	302	10.746	19.91	15.187	1.00	23.86
714	N	ILE	A	303	12.014	21.71	15.613	1.00	23.98
715	CA	ILE	A	303	13.179	20.89	15.932	1.00	22.06
716	CB	ILE	A	303	14.503	21.67	15.776	1.00	21.52
717	CG2	ILE	A	303	15.675	20.77	16.168	1.00	20.29
718	CG1	ILE	A	303	14.681	22.13	14.325	1.00	18.78
719	CD1	ILE	A	303	15.946	22.93	14.104	1.00	20.43
720	C	ILE	A	303	13.059	20.45	17.386	1.00	23.55
721	O	ILE	A	303	13.018	21.28	18.292	1.00	22.86
722	N	PRO	A	304	13	19.13	17.626	1.00	24.07
723	CD	PRO	A	304	13.119	18.03	16.644	1.00	23.94
724	CA	PRO	A	304	12.883	18.59	18.985	1.00	24.71
725	CB	PRO	A	304	13.275	17.13	18.804	1.00	24.70
726	CG	PRO	A	304	12.711	16.82	17.456	1.00	25.44
727	C	PRO	A	304	13.761	19.3	20.013	1.00	24.62
728	O	PRO	A	304	14.987	19.33	19.878	1.00	25.02
729	N	ALA	A	305	13.115	19.88	21.026	1.00	23.49
730	CA	ALA	A	305	13.788	20.58	22.124	1.00	23.80
731	CB	ALA	A	305	15.122	19.91	22.432	1.00	26.87
732	C	ALA	A	305	13.995	22.08	21.959	1.00	22.79
733	O	ALA	A	305	14.242	22.78	22.945	1.00	21.27
734	N	PHE	A	306	13.903	22.58	20.732	1.00	22.01
735	CA	PHE	A	306	14.101	24.01	20.515	1.00	22.24
736	CB	PHE	A	306	14.015	24.35	19.023	1.00	21.13
737	CG	PHE	A	306	14.301	25.8	18.714	1.00	20.73
738	CD1	PHE	A	306	13.293	26.76	18.775	1.00	21.28
739	CD2	PHE	A	306	15.591	26.21	18.393	1.00	20.25
740	CE1	PHE	A	306	13.568	28.1	18.519	1.00	20.90
741	CE2	PHE	A	306	15.875	27.55	18.136	1.00	19.14

742	CZ	PHE	A	306	14.864	28.5	18.199	1.00	19.75
743	C	PHE	A	306	13.088	24.85	21.285	1.00	22.26
744	O	PHE	A	306	13.448	25.84	21.936	1.00	22.51
745	N	ALA	A	307	11.821	24.46	21.215	1.00	23.86
746	CA	ALA	A	307	10.763	25.21	21.89	1.00	24.65
747	CB	ALA	A	307	9.399	24.7	21.441	1.00	25.58
748	C	ALA	A	307	10.868	25.16	23.413	1.00	25.96
749	O	ALA	A	307	10.238	25.96	24.102	1.00	26.50
750	N	ASN	A	308	11.667	24.23	23.932	1.00	26.32
751	CA	ASN	A	308	11.852	24.09	25.378	1.00	26.91
752	CB	ASN	A	308	12.291	22.67	25.717	1.00	27.32
753	CG	ASN	A	308	11.194	21.65	25.5	1.00	27.93
754	OD1	ASN	A	308	11.455	20.45	25.428	1.00	31.25
755	ND2	ASN	A	308	9.958	22.12	25.402	1.00	27.97
756	C	ASN	A	308	12.889	25.07	25.921	1.00	27.12
757	O	ASN	A	308	12.985	25.29	27.132	1.00	26.42
758	N	LEU	A	309	13.68	25.64	25.025	1.00	24.59
759	CA	LEU	A	309	14.702	26.6	25.428	1.00	23.00
760	CB	LEU	A	309	15.615	26.92	24.245	1.00	20.53
761	CG	LEU	A	309	16.484	25.8	23.676	1.00	20.80
762	CD1	LEU	A	309	17.175	26.3	22.414	1.00	20.69
763	CD2	LEU	A	309	17.512	25.37	24.714	1.00	21.60
764	C	LEU	A	309	14.041	27.87	25.91	1.00	21.59
765	O	LEU	A	309	12.89	28.13	25.582	1.00	20.49
766	N	ASP	A	310	14.767	28.65	26.701	1.00	23.45
767	CA	ASP	A	310	14.243	29.93	27.175	1.00	23.40
768	CB	ASP	A	310	15.263	30.64	28.062	1.00	22.34
769	CG	ASP	A	310	14.85	32.06	28.402	1.00	23.70
770	OD1	ASP	A	310	13.85	32.23	29.127	1.00	24.73
771	OD2	ASP	A	310	15.52	33	27.937	1.00	24.97
772	C	ASP	A	310	14.044	30.73	25.898	1.00	23.49
773	O	ASP	A	310	14.814	30.58	24.952	1.00	22.64
774	N	LEU	A	311	13.029	31.59	25.866	1.00	24.03
775	CA	LEU	A	311	12.762	32.38	24.669	1.00	24.61

776	CB	LEU	A	311	11.489	33.21	24.848	1.00	25.91
777	CG	LEU	A	311	11.312	34.15	26.038	1.00	29.90
778	CD1	LEU	A	311	12.37	35.25	26.043	1.00	31.19
779	CD2	LEU	A	311	9.925	34.77	25.94	1.00	32.22
780	C	LEU	A	311	13.916	33.28	24.225	1.00	23.78
781	O	LEU	A	311	14.075	33.54	23.035	1.00	22.46
782	N	ASN	A	312	14.713	33.77	25.17	1.00	22.87
783	CA	ASN	A	312	15.843	34.62	24.815	1.00	23.57
784	CB	ASN	A	312	16.501	35.19	26.072	1.00	24.41
785	CG	ASN	A	312	15.594	36.15	26.819	1.00	25.82
786	OD1	ASN	A	312	15.333	37.27	26.359	1.00	24.76
787	ND2	ASN	A	312	15.1	35.72	27.975	1.00	25.85
788	C	ASN	A	312	16.859	33.79	24.029	1.00	23.03
789	O	ASN	A	312	17.48	34.28	23.077	1.00	22.95
790	N	ASP	A	313	17.026	32.54	24.433	1.00	21.92
791	CA	ASP	A	313	17.959	31.66	23.751	1.00	21.37
792	CB	ASP	A	313	18.224	30.41	24.582	1.00	20.90
793	CG	ASP	A	313	19.281	30.63	25.649	1.00	20.90
794	OD1	ASP	A	313	19.785	31.77	25.768	1.00	22.16
795	OD2	ASP	A	313	19.609	29.67	26.364	1.00	22.62
796	C	ASP	A	313	17.411	31.28	22.383	1.00	20.42
797	O	ASP	A	313	18.176	31.07	21.442	1.00	21.27
798	N	GLN	A	314	16.088	31.2	22.268	1.00	19.98
799	CA	GLN	A	314	15.478	30.87	20.981	1.00	20.73
800	CB	GLN	A	314	13.971	30.64	21.124	1.00	20.41
801	CG	GLN	A	314	13.598	29.36	21.862	1.00	22.80
802	CD	GLN	A	314	12.1	29.12	21.906	1.00	24.47
803	OE1	GLN	A	314	11.425	29.14	20.876	1.00	26.99
804	NE2	GLN	A	314	11.571	28.89	23.104	1.00	23.97
805	C	GLN	A	314	15.74	32.04	20.03	1.00	19.47
806	O	GLN	A	314	16.099	31.84	18.869	1.00	19.20
807	N	VAL	A	315	15.561	33.25	20.541	1.00	19.92
808	CA	VAL	A	315	15.788	34.46	19.76	1.00	18.92
809	CB	VAL	A	315	15.414	35.72	20.583	1.00	19.64

810	CG1	VAL	A	315	15.861	36.98	19.867	1.00	20.62
811	CG2	VAL	A	315	13.91	35.75	20.794	1.00	19.50
812	C	VAL	A	315	17.246	34.55	19.321	1.00	18.13
813	O	VAL	A	315	17.538	34.84	18.157	1.00	17.71
814	N	THR	A	316	18.161	34.3	20.252	1.00	17.09
815	CA	THR	A	316	19.588	34.36	19.956	1.00	17.05
816	CB	THR	A	316	20.429	34.13	21.242	1.00	17.63
817	OG1	THR	A	316	20.162	35.19	22.17	1.00	16.06
818	CG2	THR	A	316	21.922	34.12	20.92	1.00	16.45
819	C	THR	A	316	20.007	33.34	18.889	1.00	16.61
820	O	THR	A	316	20.768	33.67	17.984	1.00	17.34
821	N	LEU	A	317	19.503	32.12	18.989	1.00	15.88
822	CA	LEU	A	317	19.864	31.09	18.018	1.00	16.20
823	CB	LEU	A	317	19.264	29.74	18.41	1.00	17.78
824	CG	LEU	A	317	19.886	29.11	19.656	1.00	16.63
825	CD1	LEU	A	317	19.277	27.73	19.916	1.00	17.89
826	CD2	LEU	A	317	21.393	29.01	19.46	1.00	17.96
827	C	LEU	A	317	19.417	31.48	16.616	1.00	16.44
828	O	LEU	A	317	20.147	31.27	15.643	1.00	17.08
829	N	LEU	A	318	18.221	32.05	16.507	1.00	16.59
830	CA	LEU	A	318	17.723	32.47	15.2	1.00	17.03
831	CB	LEU	A	318	16.209	32.72	15.255	1.00	16.97
832	CG	LEU	A	318	15.374	31.43	15.321	1.00	18.35
833	CD1	LEU	A	318	13.916	31.77	15.589	1.00	23.00
834	CD2	LEU	A	318	15.506	30.66	14.012	1.00	19.92
835	C	LEU	A	318	18.447	33.73	14.753	1.00	17.00
836	O	LEU	A	318	18.831	33.86	13.591	1.00	17.06
837	N	LYS	A	319	18.645	34.67	15.677	1.00	16.85
838	CA	LYS	A	319	19.332	35.91	15.335	1.00	17.88
839	CB	LYS	A	319	19.569	36.75	16.592	1.00	19.60
840	CG	LYS	A	319	20.244	38.09	16.315	1.00	21.39
841	CD	LYS	A	319	20.632	38.78	17.621	1.00	24.10
842	CE	LYS	A	319	21.26	40.14	17.374	1.00	24.44
843	NZ	LYS	A	319	20.287	41.09	16.751	1.00	26.22

844	C	LYS	A	319	20.671	35.66	14.634	1.00	18.39
845	O	LYS	A	319	20.961	36.28	13.609	1.00	19.24
846	N	TYR	A	320	21.475	34.75	15.177	1.00	16.44
847	CA	TYR	A	320	22.786	34.46	14.604	1.00	19.84
848	CB	TYR	A	320	23.781	34.13	15.721	1.00	23.67
849	CG	TYR	A	320	24.134	35.33	16.576	1.00	27.71
850	CD1	TYR	A	320	24.989	36.32	16.1	1.00	30.38
851	CE1	TYR	A	320	25.301	37.44	16.877	1.00	32.19
852	CD2	TYR	A	320	23.598	35.48	17.852	1.00	30.97
853	CE2	TYR	A	320	23.902	36.59	18.638	1.00	33.09
854	CZ	TYR	A	320	24.756	37.56	18.143	1.00	33.75
855	OH	TYR	A	320	25.075	38.65	18.916	1.00	36.85
856	C	TYR	A	320	22.8	33.33	13.577	1.00	17.92
857	O	TYR	A	320	23.708	33.26	12.747	1.00	20.86
858	N	GLY	A	321	21.795	32.47	13.612	1.00	16.75
859	CA	GLY	A	321	21.784	31.36	12.67	1.00	15.82
860	C	GLY	A	321	20.981	31.51	11.39	1.00	16.03
861	O	GLY	A	321	21.28	30.84	10.403	1.00	16.07
862	N	VAL	A	322	19.974	32.38	11.371	1.00	15.36
863	CA	VAL	A	322	19.162	32.5	10.167	1.00	16.30
864	CB	VAL	A	322	17.978	33.5	10.34	1.00	17.29
865	CG1	VAL	A	322	18.478	34.9	10.603	1.00	16.70
866	CG2	VAL	A	322	17.11	33.48	9.099	1.00	23.41
867	C	VAL	A	322	19.91	32.81	8.876	1.00	14.96
868	O	VAL	A	322	19.64	32.2	7.846	1.00	12.97
869	N	TYR	A	323	20.859	33.74	8.9	1.00	13.63
870	CA	TYR	A	323	21.544	34.05	7.651	1.00	14.50
871	CB	TYR	A	323	22.214	35.43	7.723	1.00	15.24
872	CG	TYR	A	323	21.209	36.52	7.416	1.00	15.95
873	CD1	TYR	A	323	20.791	36.76	6.108	1.00	16.47
874	CE1	TYR	A	323	19.768	37.66	5.83	1.00	17.10
875	CD2	TYR	A	323	20.586	37.23	8.446	1.00	15.91
876	CE2	TYR	A	323	19.569	38.14	8.182	1.00	15.61
877	CZ	TYR	A	323	19.161	38.35	6.875	1.00	16.58

878	OH	TYR	A	323	18.132	39.23	6.612	1.00	17.94
879	C	TYR	A	323	22.515	32.97	7.209	1.00	14.15
880	O	TYR	A	323	22.781	32.82	6.013	1.00	14.15
881	N	GLU	A	324	23.044	32.2	8.155	1.00	12.79
882	CA	GLU	A	324	23.94	31.11	7.77	1.00	13.63
883	CB	GLU	A	324	24.584	30.47	9.003	1.00	15.05
884	CG	GLU	A	324	25.608	31.38	9.689	1.00	15.42
885	CD	GLU	A	324	26.289	30.74	10.886	1.00	16.70
886	OE1	GLU	A	324	26.102	29.53	11.119	1.00	17.95
887	OE2	GLU	A	324	27.021	31.46	11.592	1.00	16.57
888	C	GLU	A	324	23.055	30.1	7.031	1.00	14.04
889	O	GLU	A	324	23.448	29.55	6.004	1.00	12.76
890	N	ALA	A	325	21.842	29.9	7.545	1.00	13.17
891	CA	ALA	A	325	20.904	28.96	6.931	1.00	13.03
892	CB	ALA	A	325	19.699	28.73	7.849	1.00	13.75
893	C	ALA	A	325	20.434	29.49	5.59	1.00	13.24
894	O	ALA	A	325	20.326	28.75	4.614	1.00	12.79
895	N	ILE	A	326	20.147	30.79	5.542	1.00	12.44
896	CA	ILE	A	326	19.692	31.4	4.306	1.00	11.19
897	CB	ILE	A	326	19.357	32.9	4.539	1.00	10.99
898	CG2	ILE	A	326	19.216	33.64	3.204	1.00	11.43
899	CG1	ILE	A	326	18.052	33	5.334	1.00	12.81
900	CD1	ILE	A	326	17.703	34.41	5.773	1.00	13.13
901	C	ILE	A	326	20.718	31.24	3.185	1.00	12.02
902	O	ILE	A	326	20.374	30.82	2.082	1.00	12.18
903	N	PHE	A	327	21.979	31.57	3.451	1.00	13.30
904	CA	PHE	A	327	22.982	31.43	2.395	1.00	13.60
905	CB	PHE	A	327	24.275	32.14	2.801	1.00	14.04
906	CG	PHE	A	327	24.093	33.61	3.059	1.00	13.96
907	CD1	PHE	A	327	23.199	34.36	2.295	1.00	16.84
908	CD2	PHE	A	327	24.819	34.25	4.054	1.00	15.29
909	CE1	PHE	A	327	23.028	35.73	2.519	1.00	17.71
910	CE2	PHE	A	327	24.657	35.62	4.284	1.00	18.04
911	CZ	PHE	A	327	23.755	36.35	3.511	1.00	15.92

912	C	PHE	A	327	23.232	29.96	2.027	1.00	13.74
913	O	PHE	A	327	23.537	29.64	0.878	1.00	13.80
914	N	ALA	A	328	23.104	29.05	2.994	1.00	13.03
915	CA	ALA	A	328	23.274	27.63	2.701	1.00	12.43
916	CB	ALA	A	328	23.255	26.8	4.003	1.00	11.53
917	C	ALA	A	328	22.127	27.18	1.783	1.00	13.70
918	O	ALA	A	328	22.342	26.48	0.788	1.00	13.68
919	N	MET	A	329	20.905	27.61	2.105	1.00	12.83
920	CA	MET	A	329	19.753	27.23	1.293	1.00	11.87
921	CB	MET	A	329	18.444	27.43	2.073	1.00	14.42
922	CG	MET	A	329	18.372	26.58	3.35	1.00	16.28
923	SD	MET	A	329	16.756	26.61	4.147	1.00	18.54
924	CE	MET	A	329	16.622	28.35	4.55	1.00	20.41
925	C	MET	A	329	19.691	27.94	-0.056	1.00	13.87
926	O	MET	A	329	19.027	27.47	-0.973	1.00	12.13
927	N	LEU	A	330	20.378	29.08	-0.193	1.00	13.97
928	CA	LEU	A	330	20.373	29.77	-1.484	1.00	15.41
929	CB	LEU	A	330	21.225	31.05	-1.43	1.00	15.37
930	CG	LEU	A	330	20.549	32.29	-0.84	1.00	18.20
931	CD1	LEU	A	330	21.486	33.49	-0.972	1.00	19.32
932	CD2	LEU	A	330	19.227	32.56	-1.56	1.00	18.93
933	C	LEU	A	330	20.934	28.85	-2.557	1.00	13.60
934	O	LEU	A	330	20.493	28.86	-3.707	1.00	15.79
935	N	SER	A	331	21.921	28.05	-2.167	1.00	12.99
936	CA	SER	A	331	22.574	27.11	-3.073	1.00	14.61
937	CB	SER	A	331	23.539	26.23	-2.277	1.00	14.55
938	OG	SER	A	331	24.355	27.04	-1.445	1.00	15.05
939	C	SER	A	331	21.553	26.24	-3.8	1.00	15.16
940	O	SER	A	331	21.739	25.88	-4.966	1.00	16.58
941	N	SER	A	332	20.474	25.89	-3.105	1.00	14.05
942	CA	SER	A	332	19.441	25.04	-3.685	1.00	14.37
943	CB	SER	A	332	18.391	24.7	-2.63	1.00	16.17
944	OG	SER	A	332	18.992	24.05	-1.527	1.00	14.97
945	C	SER	A	332	18.744	25.67	-4.889	1.00	15.39

946	O	SER	A	332	18.262	24.95	-5.768	1.00	15.48
947	N	VAL	A	333	18.677	26.99	-4.925	1.00	16.08
948	CA	VAL	A	333	18.002	27.67	-6.023	1.00	16.93
949	CB	VAL	A	333	16.985	28.72	-5.502	1.00	18.06
950	CG1	VAL	A	333	15.878	28.03	-4.717	1.00	20.27
951	CG2	VAL	A	333	17.692	29.76	-4.636	1.00	19.05
952	C	VAL	A	333	18.968	28.36	-6.971	1.00	16.26
953	O	VAL	A	333	18.55	29.14	-7.819	1.00	17.98
954	N	MET	A	334	20.253	28.03	-6.85	1.00	16.16
955	CA	MET	A	334	21.277	28.65	-7.697	1.00	17.20
956	CB	MET	A	334	22.358	29.32	-6.844	1.00	16.55
957	CG	MET	A	334	21.95	30.52	-6.005	1.00	16.51
958	SD	MET	A	334	23.363	31.08	-4.983	1.00	17.83
959	CE	MET	A	334	22.981	32.82	-4.792	1.00	19.15
960	C	MET	A	334	22.02	27.67	-8.596	1.00	19.13
961	O	MET	A	334	22.099	26.47	-8.312	1.00	20.24
962	N	ASN	A	335	22.555	28.19	-9.694	1.00	19.31
963	CA	ASN	A	335	23.426	27.42	-10.57	1.00	20.10
964	CB	ASN	A	335	22.721	26.85	-11.81	1.00	21.23
965	CG	ASN	A	335	22.146	27.9	-12.73	1.00	20.10
966	OD1	ASN	A	335	22.65	29.02	-12.83	1.00	21.27
967	ND2	ASN	A	335	21.089	27.53	-13.45	1.00	23.09
968	C	ASN	A	335	24.501	28.46	-10.9	1.00	21.45
969	O	ASN	A	335	24.433	29.58	-10.42	1.00	19.65
970	N	LYS	A	336	25.49	28.1	-11.71	1.00	21.83
971	CA	LYS	A	336	26.563	29.04	-12.01	1.00	23.64
972	CB	LYS	A	336	27.652	28.36	-12.84	1.00	26.31
973	CG	LYS	A	336	27.281	28.12	-14.3	1.00	30.33
974	CD	LYS	A	336	28.501	27.65	-15.09	1.00	34.09
975	CE	LYS	A	336	28.258	27.65	-16.6	1.00	36.35
976	NZ	LYS	A	336	27.211	26.68	-17.02	1.00	39.18
977	C	LYS	A	336	26.161	30.34	-12.7	1.00	22.90
978	O	LYS	A	336	26.927	31.31	-12.67	1.00	22.33
979	N	ASP	A	337	24.968	30.39	-13.28	1.00	21.50

980	CA	ASP	A	337	24.547	31.58	-14.01	1.00	21.46
981	CB	ASP	A	337	24.108	31.19	-15.42	1.00	22.79
982	CG	ASP	A	337	25.223	30.54	-16.21	1.00	24.81
983	OD1	ASP	A	337	26.326	31.12	-16.28	1.00	28.16
984	OD2	ASP	A	337	24.997	29.45	-16.76	1.00	26.38
985	C	ASP	A	337	23.466	32.47	-13.4	1.00	19.81
986	O	ASP	A	337	23.137	33.51	-13.96	1.00	18.99
987	N	GLY	A	338	22.91	32.06	-12.26	1.00	18.40
988	CA	GLY	A	338	21.877	32.88	-11.65	1.00	17.35
989	C	GLY	A	338	21.094	32.14	-10.58	1.00	16.28
990	O	GLY	A	338	21.473	31.04	-10.18	1.00	15.47
991	N	MET	A	339	20.001	32.74	-10.13	1.00	17.05
992	CA	MET	A	339	19.183	32.11	-9.093	1.00	17.55
993	CB	MET	A	339	19.562	32.65	-7.705	1.00	19.90
994	CG	MET	A	339	19.227	34.1	-7.44	1.00	22.04
995	SD	MET	A	339	19.422	34.52	-5.667	1.00	24.36
996	CE	MET	A	339	17.862	34.13	-5.025	1.00	23.38
997	C	MET	A	339	17.69	32.3	-9.315	1.00	17.11
998	O	MET	A	339	17.25	33.26	-9.943	1.00	17.45
999	N	LEU	A	340	16.91	31.35	-8.803	1.00	16.64
1000	CA	LEU	A	340	15.462	31.41	-8.914	1.00	16.30
1001	CB	LEU	A	340	14.848	30.05	-8.591	1.00	17.42
1002	CG	LEU	A	340	15.023	28.95	-9.62	1.00	19.04
1003	CD1	LEU	A	340	14.407	27.65	-9.08	1.00	18.84
1004	CD2	LEU	A	340	14.353	29.37	-10.92	1.00	17.82
1005	C	LEU	A	340	14.93	32.41	-7.908	1.00	16.49
1006	O	LEU	A	340	15.41	32.46	-6.776	1.00	17.61
1007	N	VAL	A	341	13.937	33.2	-8.314	1.00	14.86
1008	CA	VAL	A	341	13.333	34.17	-7.42	1.00	15.11
1009	CB	VAL	A	341	13.879	35.61	-7.673	1.00	14.89
1010	CG1	VAL	A	341	15.402	35.61	-7.55	1.00	17.85
1011	CG2	VAL	A	341	13.446	36.11	-9.045	1.00	16.47
1012	C	VAL	A	341	11.821	34.19	-7.593	1.00	14.36
1013	O	VAL	A	341	11.279	33.55	-8.499	1.00	15.87

1014	N	ALA	A	342	11.15	34.93	-6.717	1.00	13.97
1015	CA	ALA	A	342	9.701	35.07	-6.753	1.00	14.91
1016	CB	ALA	A	342	9.29	35.9	-7.966	1.00	15.58
1017	C	ALA	A	342	8.981	33.72	-6.768	1.00	14.63
1018	O	ALA	A	342	8.176	33.44	-7.664	1.00	14.60
1019	N	TYR	A	343	9.281	32.9	-5.769	1.00	14.26
1020	CA	TYR	A	343	8.655	31.59	-5.627	1.00	15.27
1021	CB	TYR	A	343	7.191	31.78	-5.224	1.00	15.76
1022	CG	TYR	A	343	7.085	32.36	-3.832	1.00	18.04
1023	CD1	TYR	A	343	7.013	31.53	-2.715	1.00	19.51
1024	CE1	TYR	A	343	7.059	32.05	-1.422	1.00	20.29
1025	CD2	TYR	A	343	7.191	33.74	-3.626	1.00	19.02
1026	CE2	TYR	A	343	7.245	34.27	-2.339	1.00	20.93
1027	CZ	TYR	A	343	7.183	33.43	-1.244	1.00	20.76
1028	OH	TYR	A	343	7.283	33.95	0.027	1.00	21.61
1029	C	TYR	A	343	8.791	30.72	-6.869	1.00	14.54
1030	O	TYR	A	343	7.847	30.04	-7.289	1.00	15.22
1031	N	GLY	A	344	9.991	30.75	-7.439	1.00	15.09
1032	CA	GLY	A	344	10.308	29.95	-8.61	1.00	16.73
1033	C	GLY	A	344	9.804	30.45	-9.945	1.00	18.37
1034	O	GLY	A	344	9.989	29.78	-10.96	1.00	18.69
1035	N	ASN	A	345	9.187	31.63	-9.969	1.00	18.57
1036	CA	ASN	A	345	8.659	32.13	-11.23	1.00	18.81
1037	CB	ASN	A	345	7.317	32.82	-11	1.00	21.87
1038	CG	ASN	A	345	6.156	31.83	-11	1.00	24.72
1039	OD1	ASN	A	345	5.003	32.23	-10.97	1.00	32.52
1040	ND2	ASN	A	345	6.465	30.55	-11.03	1.00	29.15
1041	C	ASN	A	345	9.596	33.06	-11.99	1.00	18.54
1042	O	ASN	A	345	9.275	33.49	-13.09	1.00	16.73
1043	N	GLY	A	346	10.75	33.34	-11.41	1.00	16.20
1044	CA	GLY	A	346	11.716	34.19	-12.07	1.00	16.52
1045	C	GLY	A	346	13.11	33.64	-11.89	1.00	16.47
1046	O	GLY	A	346	13.336	32.8	-11.01	1.00	15.40
1047	N	PHE	A	347	14.042	34.09	-12.73	1.00	15.82

1048	CA	PHE	A	347	15.435	33.66	-12.65	1.00	15.40
1049	CB	PHE	A	347	15.719	32.53	-13.65	1.00	16.65
1050	CG	PHE	A	347	17.154	32.06	-13.64	1.00	20.70
1051	CD1	PHE	A	347	18.106	32.65	-14.48	1.00	19.82
1052	CD2	PHE	A	347	17.553	31.02	-12.81	1.00	19.54
1053	CE1	PHE	A	347	19.427	32.21	-14.48	1.00	22.34
1054	CE2	PHE	A	347	18.879	30.57	-12.8	1.00	22.09
1055	CZ	PHE	A	347	19.817	31.17	-13.63	1.00	22.09
1056	C	PHE	A	347	16.261	34.9	-13	1.00	16.41
1057	O	PHE	A	347	16.199	35.4	-14.12	1.00	15.80
1058	N	ILE	A	348	17.012	35.39	-12.02	1.00	14.27
1059	CA	ILE	A	348	17.825	36.58	-12.24	1.00	15.49
1060	CB	ILE	A	348	17.683	37.55	-11.03	1.00	15.76
1061	CG2	ILE	A	348	18.184	36.9	-9.764	1.00	17.30
1062	CG1	ILE	A	348	18.433	38.85	-11.31	1.00	15.24
1063	CD1	ILE	A	348	17.966	40	-10.42	1.00	16.30
1064	C	ILE	A	348	19.272	36.15	-12.46	1.00	16.57
1065	O	ILE	A	348	19.833	35.38	-11.68	1.00	16.99
1066	N	THR	A	349	19.884	36.65	-13.53	1.00	15.69
1067	CA	THR	A	349	21.254	36.24	-13.83	1.00	17.54
1068	CB	THR	A	349	21.628	36.5	-15.32	1.00	18.08
1069	OG1	THR	A	349	21.684	37.91	-15.57	1.00	18.08
1070	CG2	THR	A	349	20.615	35.86	-16.23	1.00	19.40
1071	C	THR	A	349	22.34	36.85	-12.97	1.00	17.79
1072	O	THR	A	349	22.279	38.01	-12.56	1.00	17.03
1073	N	ARG	A	350	23.344	36.02	-12.72	1.00	18.29
1074	CA	ARG	A	350	24.501	36.39	-11.94	1.00	20.41
1075	CB	ARG	A	350	25.467	35.21	-11.91	1.00	20.86
1076	CG	ARG	A	350	26.714	35.44	-11.11	1.00	23.49
1077	CD	ARG	A	350	27.498	34.15	-11.01	1.00	22.29
1078	NE	ARG	A	350	28.617	34.28	-10.09	1.00	25.39
1079	CZ	ARG	A	350	29.426	33.28	-9.755	1.00	25.74
1080	NH1	ARG	A	350	29.237	32.07	-10.26	1.00	25.82
1081	NH2	ARG	A	350	30.417	33.5	-8.906	1.00	25.63

1082	C	ARG	A	350	25.173	37.61	-12.58	1.00	20.85
1083	O	ARG	A	350	25.624	38.52	-11.89	1.00	20.39
1084	N	GLU	A	351	25.226	37.61	-13.91	1.00	21.71
1085	CA	GLU	A	351	25.86	38.71	-14.63	1.00	23.42
1086	CB	GLU	A	351	26.045	38.34	-16.1	1.00	26.93
1087	CG	GLU	A	351	27.152	37.31	-16.32	1.00	31.26
1088	CD	GLU	A	351	28.504	37.81	-15.83	1.00	33.51
1089	OE1	GLU	A	351	28.97	38.86	-16.3	1.00	36.23
1090	OE2	GLU	A	351	29.103	37.14	-14.96	1.00	36.72
1091	C	GLU	A	351	25.106	40.04	-14.51	1.00	21.78
1092	O	GLU	A	351	25.723	41.1	-14.42	1.00	23.51
1093	N	PHE	A	352	23.779	39.98	-14.49	1.00	20.79
1094	CA	PHE	A	352	22.988	41.19	-14.35	1.00	20.13
1095	CB	PHE	A	352	21.496	40.88	-14.53	1.00	21.21
1096	CG	PHE	A	352	20.603	42.07	-14.3	1.00	22.31
1097	CD1	PHE	A	352	20.806	43.26	-14.99	1.00	22.58
1098	CD2	PHE	A	352	19.561	42	-13.38	1.00	22.12
1099	CE1	PHE	A	352	19.985	44.36	-14.77	1.00	22.50
1100	CE2	PHE	A	352	18.734	43.1	-13.15	1.00	21.07
1101	CZ	PHE	A	352	18.947	44.28	-13.85	1.00	23.38
1102	C	PHE	A	352	23.246	41.79	-12.97	1.00	20.06
1103	O	PHE	A	352	23.411	43	-12.82	1.00	18.10
1104	N	LEU	A	353	23.291	40.93	-11.95	1.00	19.09
1105	CA	LEU	A	353	23.537	41.39	-10.6	1.00	19.98
1106	CB	LEU	A	353	23.431	40.22	-9.622	1.00	18.81
1107	CG	LEU	A	353	21.998	39.71	-9.458	1.00	17.36
1108	CD1	LEU	A	353	22.019	38.3	-8.885	1.00	17.66
1109	CD2	LEU	A	353	21.208	40.67	-8.55	1.00	18.64
1110	C	LEU	A	353	24.895	42.08	-10.45	1.00	20.25
1111	O	LEU	A	353	25.003	43.12	-9.792	1.00	20.17
1112	N	LYS	A	354	25.931	41.53	-11.07	1.00	22.58
1113	CA	LYS	A	354	27.248	42.15	-10.97	1.00	25.12
1114	CB	LYS	A	354	28.334	41.15	-11.39	1.00	28.30
1115	CG	LYS	A	354	28.091	40.46	-12.71	1.00	31.49

1116	CD	LYS	A	354	28.929	39.19	-12.83	1.00	34.20
1117	CE	LYS	A	354	30.416	39.46	-12.65	1.00	32.93
1118	NZ	LYS	A	354	31.234	38.26	-12.95	1.00	33.54
1119	C	LYS	A	354	27.349	43.45	-11.77	1.00	26.38
1120	O	LYS	A	354	28.23	44.28	-11.51	1.00	28.05
1121	N	SER	A	355	26.425	43.64	-12.71	1.00	25.99
1122	CA	SER	A	355	26.404	44.84	-13.55	1.00	25.78
1123	CB	SER	A	355	25.604	44.6	-14.83	1.00	27.38
1124	OG	SER	A	355	24.213	44.75	-14.59	1.00	27.61
1125	C	SER	A	355	25.786	46.03	-12.82	1.00	25.54
1126	O	SER	A	355	25.874	47.17	-13.28	1.00	24.80
1127	N	LEU	A	356	25.148	45.76	-11.69	1.00	21.74
1128	CA	LEU	A	356	24.524	46.82	-10.92	1.00	21.47
1129	CB	LEU	A	356	23.682	46.23	-9.789	1.00	20.68
1130	CG	LEU	A	356	22.535	45.31	-10.21	1.00	17.94
1131	CD1	LEU	A	356	21.93	44.68	-8.965	1.00	17.43
1132	CD2	LEU	A	356	21.487	46.11	-10.99	1.00	18.91
1133	C	LEU	A	356	25.576	47.75	-10.34	1.00	22.34
1134	O	LEU	A	356	26.765	47.43	-10.3	1.00	21.32
1135	N	ARG	A	357	25.115	48.9	-9.876	1.00	23.03
1136	CA	ARG	A	357	25.973	49.9	-9.272	1.00	24.90
1137	CB	ARG	A	357	25.177	51.21	-9.192	1.00	26.16
1138	CG	ARG	A	357	25.46	52.09	-7.996	1.00	28.63
1139	CD	ARG	A	357	24.766	53.44	-8.141	1.00	27.93
1140	NE	ARG	A	357	23.501	53.56	-7.416	1.00	25.84
1141	CZ	ARG	A	357	23.381	53.49	-6.094	1.00	25.53
1142	NH1	ARG	A	357	24.449	53.28	-5.332	1.00	26.92
1143	NH2	ARG	A	357	22.199	53.68	-5.527	1.00	26.63
1144	C	ARG	A	357	26.422	49.46	-7.879	1.00	23.21
1145	O	ARG	A	357	25.675	48.78	-7.177	1.00	22.61
1146	N	LYS	A	358	27.646	49.81	-7.483	1.00	23.12
1147	CA	LYS	A	358	28.109	49.46	-6.141	1.00	22.49
1148	CB	LYS	A	358	29.576	49.87	-5.923	1.00	23.58
1149	CG	LYS	A	358	30.609	49.05	-6.695	1.00	22.91

1150	CD	LYS	A	358	32.035	49.59	-6.461	1.00	25.76
1151	CE	LYS	A	358	32.702	48.99	-5.225	1.00	26.68
1152	NZ	LYS	A	358	33.206	47.61	-5.476	1.00	28.29
1153	C	LYS	A	358	27.219	50.27	-5.198	1.00	22.76
1154	O	LYS	A	358	26.764	51.36	-5.548	1.00	24.51
1155	N	PRO	A	359	26.982	49.76	-3.98	1.00	21.69
1156	CD	PRO	A	359	26.263	50.5	-2.93	1.00	23.55
1157	CA	PRO	A	359	27.492	48.49	-3.451	1.00	21.20
1158	CB	PRO	A	359	27.626	48.8	-1.973	1.00	23.13
1159	CG	PRO	A	359	26.366	49.56	-1.719	1.00	22.88
1160	C	PRO	A	359	26.548	47.32	-3.7	1.00	20.65
1161	O	PRO	A	359	26.81	46.19	-3.257	1.00	20.59
1162	N	PHE	A	360	25.454	47.57	-4.404	1.00	19.16
1163	CA	PHE	A	360	24.473	46.52	-4.671	1.00	18.85
1164	CB	PHE	A	360	23.25	47.14	-5.355	1.00	20.28
1165	CG	PHE	A	360	22.536	48.14	-4.492	1.00	19.94
1166	CD1	PHE	A	360	21.728	47.72	-3.435	1.00	18.19
1167	CD2	PHE	A	360	22.72	49.51	-4.692	1.00	18.89
1168	CE1	PHE	A	360	21.115	48.65	-2.586	1.00	19.37
1169	CE2	PHE	A	360	22.113	50.43	-3.851	1.00	19.54
1170	CZ	PHE	A	360	21.309	50	-2.794	1.00	19.87
1171	C	PHE	A	360	25.038	45.36	-5.473	1.00	19.99
1172	O	PHE	A	360	24.618	44.21	-5.292	1.00	19.11
1173	N	CYS	A	361	26.009	45.64	-6.338	1.00	17.57
1174	CA	CYS	A	361	26.619	44.58	-7.14	1.00	18.30
1175	CB	CYS	A	361	27.353	45.19	-8.34	1.00	18.99
1176	SG	CYS	A	361	28.657	46.36	-7.884	1.00	20.67
1177	C	CYS	A	361	27.598	43.76	-6.305	1.00	18.14
1178	O	CYS	A	361	28.112	42.75	-6.769	1.00	17.82
1179	N	ASP	A	362	27.837	44.19	-5.068	1.00	18.21
1180	CA	ASP	A	362	28.777	43.48	-4.205	1.00	18.60
1181	CB	ASP	A	362	29.631	44.49	-3.435	1.00	20.06
1182	CG	ASP	A	362	30.428	45.4	-4.359	1.00	20.29
1183	OD1	ASP	A	362	31.017	44.88	-5.319	1.00	21.00

1184	OD2	ASP	A	362	30.464	46.62	-4.121	1.00	22.31
1185	C	ASP	A	362	28.105	42.54	-3.22	1.00	19.14
1186	O	ASP	A	362	28.767	41.93	-2.374	1.00	20.18
1187	N	ILE	A	363	26.791	42.41	-3.344	1.00	17.15
1188	CA	ILE	A	363	26.021	41.56	-2.446	1.00	18.64
1189	CB	ILE	A	363	24.536	42	-2.418	1.00	19.28
1190	CG2	ILE	A	363	23.729	41.06	-1.525	1.00	17.16
1191	CG1	ILE	A	363	24.424	43.44	-1.922	1.00	19.43
1192	CD1	ILE	A	363	23.004	43.98	-1.928	1.00	19.79
1193	C	ILE	A	363	26.039	40.08	-2.781	1.00	18.41
1194	O	ILE	A	363	26.419	39.25	-1.954	1.00	17.58
1195	N	MET	A	364	25.635	39.75	-4.002	1.00	20.04
1196	CA	MET	A	364	25.511	38.35	-4.409	1.00	18.56
1197	CB	MET	A	364	24.434	38.24	-5.491	1.00	19.49
1198	CG	MET	A	364	23.037	38.63	-5.018	1.00	20.24
1199	SD	MET	A	364	22.485	37.68	-3.579	1.00	20.20
1200	CE	MET	A	364	22.609	36.01	-4.236	1.00	16.96
1201	C	MET	A	364	26.706	37.5	-4.823	1.00	18.99
1202	O	MET	A	364	26.654	36.29	-4.644	1.00	17.53
1203	N	GLU	A	365	27.771	38.09	-5.369	1.00	19.55
1204	CA	GLU	A	365	28.91	37.27	-5.794	1.00	19.92
1205	CB	GLU	A	365	30.078	38.13	-6.287	1.00	21.97
1206	CG	GLU	A	365	30.022	38.5	-7.756	1.00	26.26
1207	CD	GLU	A	365	29.832	37.29	-8.656	1.00	27.30
1208	OE1	GLU	A	365	28.693	37.06	-9.104	1.00	26.68
1209	OE2	GLU	A	365	30.817	36.57	-8.909	1.00	29.91
1210	C	GLU	A	365	29.436	36.29	-4.748	1.00	18.52
1211	O	GLU	A	365	29.628	35.11	-5.042	1.00	18.23
1212	N	PRO	A	366	29.689	36.76	-3.516	1.00	18.98
1213	CD	PRO	A	366	29.537	38.13	-2.997	1.00	20.10
1214	CA	PRO	A	366	30.198	35.86	-2.47	1.00	19.09
1215	CB	PRO	A	366	30.29	36.78	-1.251	1.00	20.02
1216	CG	PRO	A	366	30.52	38.14	-1.862	1.00	20.53
1217	C	PRO	A	366	29.278	34.66	-2.211	1.00	17.84

1218	O	PRO	A	366	29.736	33.57	-1.851	1.00	15.96
1219	N	LYS	A	367	27.98	34.88	-2.388	1.00	17.85
1220	CA	LYS	A	367	26.992	33.82	-2.17	1.00	16.69
1221	CB	LYS	A	367	25.603	34.44	-1.964	1.00	17.55
1222	CG	LYS	A	367	25.415	35.17	-0.624	1.00	16.13
1223	CD	LYS	A	367	26.254	36.45	-0.534	1.00	18.57
1224	CE	LYS	A	367	25.819	37.34	0.626	1.00	16.06
1225	NZ	LYS	A	367	26.671	38.58	0.743	1.00	15.29
1226	C	LYS	A	367	26.963	32.84	-3.337	1.00	17.68
1227	O	LYS	A	367	26.783	31.63	-3.142	1.00	17.04
1228	N	PHE	A	368	27.127	33.35	-4.555	1.00	17.39
1229	CA	PHE	A	368	27.156	32.47	-5.719	1.00	16.62
1230	CB	PHE	A	368	27.169	33.28	-7.023	1.00	16.38
1231	CG	PHE	A	368	25.796	33.65	-7.527	1.00	18.08
1232	CD1	PHE	A	368	24.936	32.68	-8.039	1.00	17.39
1233	CD2	PHE	A	368	25.364	34.97	-7.495	1.00	16.89
1234	CE1	PHE	A	368	23.67	33.02	-8.507	1.00	17.41
1235	CE2	PHE	A	368	24.102	35.32	-7.96	1.00	16.42
1236	CZ	PHE	A	368	23.253	34.35	-8.467	1.00	16.76
1237	C	PHE	A	368	28.426	31.63	-5.6	1.00	16.15
1238	O	PHE	A	368	28.407	30.42	-5.842	1.00	16.24
1239	N	ASP	A	369	29.53	32.26	-5.206	1.00	18.27
1240	CA	ASP	A	369	30.783	31.52	-5.049	1.00	18.69
1241	CB	ASP	A	369	31.952	32.46	-4.709	1.00	20.51
1242	CG	ASP	A	369	32.444	33.24	-5.922	1.00	22.65
1243	OD1	ASP	A	369	32.327	32.72	-7.05	1.00	23.09
1244	OD2	ASP	A	369	32.959	34.36	-5.748	1.00	27.87
1245	C	ASP	A	369	30.638	30.44	-3.979	1.00	18.16
1246	O	ASP	A	369	31.117	29.32	-4.159	1.00	17.43
1247	N	PHE	A	370	29.969	30.76	-2.872	1.00	16.51
1248	CA	PHE	A	370	29.785	29.75	-1.833	1.00	17.11
1249	CB	PHE	A	370	29.146	30.33	-0.571	1.00	17.43
1250	CG	PHE	A	370	28.76	29.28	0.443	1.00	16.12
1251	CD1	PHE	A	370	27.548	28.61	0.339	1.00	15.11

1252	CD2	PHE	A	370	29.643	28.93	1.461	1.00	16.71
1253	CE1	PHE	A	370	27.219	27.58	1.231	1.00	14.11
1254	CE2	PHE	A	370	29.323	27.9	2.356	1.00	15.23
1255	CZ	PHE	A	370	28.109	27.23	2.238	1.00	11.27
1256	C	PHE	A	370	28.902	28.61	-2.342	1.00	16.98
1257	O	PHE	A	370	29.21	27.44	-2.136	1.00	16.87
1258	N	ALA	A	371	27.802	28.97	-2.995	1.00	16.32
1259	CA	ALA	A	371	26.854	27.99	-3.518	1.00	19.25
1260	CB	ALA	A	371	25.659	28.71	-4.147	1.00	17.22
1261	C	ALA	A	371	27.467	27.02	-4.529	1.00	19.60
1262	O	ALA	A	371	27.09	25.85	-4.58	1.00	20.69
1263	N	MET	A	372	28.401	27.51	-5.337	1.00	19.90
1264	CA	MET	A	372	29.029	26.66	-6.342	1.00	23.22
1265	CB	MET	A	372	29.948	27.48	-7.242	1.00	25.16
1266	CG	MET	A	372	29.599	27.38	-8.714	1.00	31.86
1267	SD	MET	A	372	27.844	27.66	-9.043	1.00	35.24
1268	CE	MET	A	372	27.242	26	-9.114	1.00	37.40
1269	C	MET	A	372	29.817	25.54	-5.671	1.00	22.48
1270	O	MET	A	372	29.732	24.38	-6.074	1.00	22.07
1271	N	LYS	A	373	30.577	25.89	-4.641	1.00	21.68
1272	CA	LYS	A	373	31.347	24.88	-3.929	1.00	22.55
1273	CB	LYS	A	373	32.445	25.56	-3.098	1.00	24.59
1274	CG	LYS	A	373	33.599	26.04	-3.977	1.00	28.52
1275	CD	LYS	A	373	34.722	26.71	-3.205	1.00	31.12
1276	CE	LYS	A	373	34.309	28.07	-2.681	1.00	33.08
1277	NZ	LYS	A	373	35.503	28.85	-2.253	1.00	34.91
1278	C	LYS	A	373	30.432	24.02	-3.059	1.00	22.72
1279	O	LYS	A	373	30.685	22.83	-2.874	1.00	22.63
1280	N	PHE	A	374	29.355	24.61	-2.545	1.00	21.24
1281	CA	PHE	A	374	28.425	23.86	-1.708	1.00	20.87
1282	CB	PHE	A	374	27.417	24.79	-1.031	1.00	19.09
1283	CG	PHE	A	374	26.647	24.15	0.097	1.00	19.22
1284	CD1	PHE	A	374	27.258	23.91	1.321	1.00	19.37
1285	CD2	PHE	A	374	25.306	23.81	-0.064	1.00	19.20

1286	CE1	PHE	A	374	26.543	23.33	2.376	1.00	18.07
1287	CE2	PHE	A	374	24.579	23.23	0.98	1.00	18.27
1288	CZ	PHE	A	374	25.2	22.99	2.203	1.00	18.45
1289	C	PHE	A	374	27.667	22.82	-2.536	1.00	20.34
1290	O	PHE	A	374	27.503	21.67	-2.115	1.00	19.46
1291	N	ASN	A	375	27.204	23.23	-3.714	1.00	20.08
1292	CA	ASN	A	375	26.458	22.35	-4.607	1.00	21.22
1293	CB	ASN	A	375	25.903	23.15	-5.791	1.00	21.85
1294	CG	ASN	A	375	24.613	23.89	-5.449	1.00	22.68
1295	OD1	ASN	A	375	24.238	24.85	-6.119	1.00	22.40
1296	ND2	ASN	A	375	23.922	23.42	-4.415	1.00	20.32
1297	C	ASN	A	375	27.322	21.2	-5.119	1.00	21.97
1298	O	ASN	A	375	26.807	20.14	-5.483	1.00	22.05
1299	N	ALA	A	376	28.632	21.41	-5.142	1.00	20.80
1300	CA	ALA	A	376	29.561	20.38	-5.597	1.00	22.52
1301	CB	ALA	A	376	30.974	20.95	-5.677	1.00	22.39
1302	C	ALA	A	376	29.52	19.2	-4.643	1.00	23.80
1303	O	ALA	A	376	30.008	18.11	-4.971	1.00	24.70
1304	N	LEU	A	377	28.943	19.4	-3.459	1.00	22.37
1305	CA	LEU	A	377	28.824	18.34	-2.466	1.00	23.08
1306	CB	LEU	A	377	28.577	18.93	-1.072	1.00	23.25
1307	CG	LEU	A	377	29.719	19.77	-0.485	1.00	23.11
1308	CD1	LEU	A	377	29.376	20.19	0.94	1.00	22.57
1309	CD2	LEU	A	377	31.001	18.95	-0.488	1.00	24.48
1310	C	LEU	A	377	27.686	17.39	-2.833	1.00	22.79
1311	O	LEU	A	377	27.549	16.31	-2.249	1.00	22.44
1312	N	GLU	A	378	26.865	17.8	-3.793	1.00	22.82
1313	CA	GLU	A	378	25.75	16.99	-4.256	1.00	24.48
1314	CB	GLU	A	378	26.291	15.74	-4.949	1.00	26.99
1315	CG	GLU	A	378	26.137	15.73	-6.449	1.00	33.00
1316	CD	GLU	A	378	26.938	14.62	-7.093	1.00	35.36
1317	OE1	GLU	A	378	27.012	13.52	-6.502	1.00	37.48
1318	OE2	GLU	A	378	27.487	14.84	-8.188	1.00	36.92
1319	C	GLU	A	378	24.786	16.57	-3.153	1.00	22.38

1320	O	GLU	A	378	24.3	15.44	-3.142	1.00	23.39
1321	N	LEU	A	379	24.511	17.47	-2.219	1.00	21.57
1322	CA	LEU	A	379	23.589	17.16	-1.134	1.00	18.06
1323	CB	LEU	A	379	23.714	18.18	-0.004	1.00	18.81
1324	CG	LEU	A	379	25.061	18.39	0.688	1.00	16.97
1325	CD1	LEU	A	379	24.863	19.34	1.858	1.00	16.61
1326	CD2	LEU	A	379	25.599	17.06	1.19	1.00	18.25
1327	C	LEU	A	379	22.153	17.19	-1.64	1.00	18.75
1328	O	LEU	A	379	21.855	17.83	-2.651	1.00	19.00
1329	N	ASP	A	380	21.273	16.48	-0.947	1.00	19.17
1330	CA	ASP	A	380	19.862	16.48	-1.296	1.00	18.60
1331	CB	ASP	A	380	19.339	15.06	-1.59	1.00	19.63
1332	CG	ASP	A	380	19.486	14.12	-0.42	1.00	21.42
1333	OD1	ASP	A	380	19.266	14.55	0.728	1.00	18.99
1334	OD2	ASP	A	380	19.801	12.93	-0.657	1.00	24.09
1335	C	ASP	A	380	19.153	17.09	-0.092	1.00	18.66
1336	O	ASP	A	380	19.791	17.39	0.917	1.00	19.31
1337	N	ASP	A	381	17.846	17.28	-0.191	1.00	18.35
1338	CA	ASP	A	381	17.097	17.9	0.894	1.00	18.08
1339	CB	ASP	A	381	15.64	18.08	0.473	1.00	20.09
1340	CG	ASP	A	381	15.489	19.09	-0.658	1.00	21.21
1341	OD1	ASP	A	381	15.934	20.25	-0.482	1.00	20.02
1342	OD2	ASP	A	381	14.932	18.73	-1.719	1.00	22.56
1343	C	ASP	A	381	17.185	17.17	2.234	1.00	17.57
1344	O	ASP	A	381	17.159	17.81	3.284	1.00	17.01
1345	N	SER	A	382	17.297	15.84	2.219	1.00	16.66
1346	CA	SER	A	382	17.403	15.13	3.49	1.00	17.74
1347	CB	SER	A	382	17.364	13.6	3.284	1.00	16.26
1348	OG	SER	A	382	18.502	13.1	2.606	1.00	18.96
1349	C	SER	A	382	18.695	15.55	4.197	1.00	17.27
1350	O	SER	A	382	18.722	15.69	5.419	1.00	19.27
1351	N	ASP	A	383	19.759	15.77	3.427	1.00	16.48
1352	CA	ASP	A	383	21.042	16.2	4.003	1.00	15.88
1353	CB	ASP	A	383	22.172	16.15	2.967	1.00	15.19

1354	CG	ASP	A	383	22.32	14.8	2.306	1.00	18.19
1355	OD1	ASP	A	383	22.365	13.78	3.025	1.00	19.73
1356	OD2	ASP	A	383	22.414	14.78	1.059	1.00	17.35
1357	C	ASP	A	383	20.944	17.64	4.494	1.00	15.34
1358	O	ASP	A	383	21.351	17.96	5.61	1.00	13.16
1359	N	ILE	A	384	20.416	18.5	3.631	1.00	14.16
1360	CA	ILE	A	384	20.279	19.92	3.925	1.00	14.77
1361	CB	ILE	A	384	19.661	20.66	2.712	1.00	14.32
1362	CG2	ILE	A	384	19.454	22.13	3.047	1.00	13.42
1363	CG1	ILE	A	384	20.594	20.52	1.508	1.00	12.81
1364	CD1	ILE	A	384	19.943	20.83	0.161	1.00	10.35
1365	C	ILE	A	384	19.452	20.19	5.18	1.00	15.58
1366	O	ILE	A	384	19.813	21.03	6.001	1.00	15.62
1367	N	SER	A	385	18.355	19.45	5.344	1.00	15.94
1368	CA	SER	A	385	17.513	19.66	6.516	1.00	17.39
1369	CB	SER	A	385	16.323	18.7	6.508	1.00	18.46
1370	OG	SER	A	385	16.747	17.36	6.665	1.00	19.88
1371	C	SER	A	385	18.313	19.48	7.799	1.00	16.76
1372	O	SER	A	385	18.146	20.24	8.735	1.00	15.46
1373	N	LEU	A	386	19.179	18.47	7.841	1.00	17.17
1374	CA	LEU	A	386	19.987	18.22	9.04	1.00	18.15
1375	CB	LEU	A	386	20.649	16.83	8.973	1.00	18.31
1376	CG	LEU	A	386	19.688	15.64	8.899	1.00	20.80
1377	CD1	LEU	A	386	20.461	14.33	8.89	1.00	22.15
1378	CD2	LEU	A	386	18.741	15.68	10.089	1.00	22.01
1379	C	LEU	A	386	21.062	19.29	9.21	1.00	17.32
1380	O	LEU	A	386	21.347	19.72	10.326	1.00	17.55
1381	N	PHE	A	387	21.655	19.7	8.094	1.00	15.68
1382	CA	PHE	A	387	22.701	20.72	8.093	1.00	15.42
1383	CB	PHE	A	387	23.191	20.94	6.658	1.00	14.83
1384	CG	PHE	A	387	24.356	21.88	6.546	1.00	17.91
1385	CD1	PHE	A	387	25.631	21.48	6.933	1.00	18.12
1386	CD2	PHE	A	387	24.174	23.17	6.06	1.00	17.17
1387	CE1	PHE	A	387	26.711	22.36	6.835	1.00	19.84

1388	CE2	PHE	A	387	25.248	24.06	5.96	1.00	17.27
1389	CZ	PHE	A	387	26.519	23.64	6.349	1.00	18.98
1390	C	PHE	A	387	22.14	22.03	8.667	1.00	14.65
1391	O	PHE	A	387	22.78	22.7	9.488	1.00	14.80
1392	N	VAL	A	388	20.937	22.4	8.235	1.00	14.52
1393	CA	VAL	A	388	20.302	23.62	8.715	1.00	13.14
1394	CB	VAL	A	388	19.061	23.96	7.856	1.00	14.31
1395	CG1	VAL	A	388	18.253	25.08	8.481	1.00	13.46
1396	CG2	VAL	A	388	19.531	24.38	6.456	1.00	13.68
1397	C	VAL	A	388	19.941	23.53	10.205	1.00	14.97
1398	O	VAL	A	388	20.1	24.5	10.946	1.00	14.16
1399	N	ALA	A	389	19.468	22.37	10.651	1.00	14.60
1400	CA	ALA	A	389	19.132	22.21	12.068	1.00	15.75
1401	CB	ALA	A	389	18.534	20.83	12.333	1.00	14.49
1402	C	ALA	A	389	20.409	22.39	12.884	1.00	17.48
1403	O	ALA	A	389	20.39	22.96	13.974	1.00	18.76
1404	N	ALA	A	390	21.516	21.89	12.345	1.00	17.47
1405	CA	ALA	A	390	22.806	21.99	13.012	1.00	18.52
1406	CB	ALA	A	390	23.838	21.13	12.278	1.00	18.08
1407	C	ALA	A	390	23.295	23.44	13.117	1.00	18.95
1408	O	ALA	A	390	23.835	23.84	14.146	1.00	18.98
1409	N	ILE	A	391	23.113	24.24	12.069	1.00	18.97
1410	CA	ILE	A	391	23.579	25.62	12.165	1.00	19.61
1411	CB	ILE	A	391	23.595	26.35	10.777	1.00	22.32
1412	CG2	ILE	A	391	24.049	25.41	9.693	1.00	22.00
1413	CG1	ILE	A	391	22.233	26.94	10.455	1.00	25.81
1414	CD1	ILE	A	391	22.036	28.31	11.06	1.00	26.92
1415	C	ILE	A	391	22.718	26.41	13.158	1.00	19.24
1416	O	ILE	A	391	23.218	27.27	13.876	1.00	18.21
1417	N	ILE	A	392	21.429	26.09	13.212	1.00	17.90
1418	CA	ILE	A	392	20.514	26.77	14.118	1.00	18.91
1419	CB	ILE	A	392	19.047	26.43	13.79	1.00	20.25
1420	CG2	ILE	A	392	18.119	26.92	14.901	1.00	20.50
1421	CG1	ILE	A	392	18.658	27.05	12.449	1.00	19.74

1422	CD1	ILE	A	392	17.232	26.77	12.028	1.00	20.27
1423	C	ILE	A	392	20.785	26.43	15.583	1.00	19.83
1424	O	ILE	A	392	20.872	27.32	16.435	1.00	18.98
1425	N	CYS	A	393	20.935	25.15	15.874	1.00	21.71
1426	CA	CYS	A	393	21.175	24.73	17.249	1.00	24.63
1427	CB	CYS	A	393	20.59	23.34	17.457	1.00	26.05
1428	SG	CYS	A	393	18.833	23.3	17.09	1.00	27.14
1429	C	CYS	A	393	22.655	24.76	17.576	1.00	25.29
1430	O	CYS	A	393	23.279	23.73	17.837	1.00	26.58
1431	N	CYS	A	394	23.196	25.97	17.561	1.00	27.00
1432	CA	CYS	A	394	24.602	26.23	17.818	1.00	28.30
1433	CB	CYS	A	394	25.095	27.25	16.792	1.00	30.14
1434	SG	CYS	A	394	26.804	27.71	16.962	1.00	32.84
1435	C	CYS	A	394	24.818	26.77	19.237	1.00	27.82
1436	O	CYS	A	394	24.279	27.82	19.602	1.00	27.12
1437	N	GLY	A	395	25.619	26.06	20.025	1.00	28.23
1438	CA	GLY	A	395	25.869	26.48	21.394	1.00	28.09
1439	C	GLY	A	395	26.924	27.55	21.575	1.00	28.17
1440	O	GLY	A	395	27.155	28.01	22.693	1.00	30.05
1441	N	ASP	A	396	27.556	27.97	20.483	1.00	29.00
1442	CA	ASP	A	396	28.603	28.98	20.54	1.00	29.78
1443	CB	ASP	A	396	29.678	28.7	19.49	1.00	33.93
1444	CG	ASP	A	396	30.174	27.28	19.544	1.00	37.57
1445	OD1	ASP	A	396	30.417	26.78	20.664	1.00	40.66
1446	OD2	ASP	A	396	30.329	26.66	18.466	1.00	39.44
1447	C	ASP	A	396	28.108	30.41	20.326	1.00	27.38
1448	O	ASP	A	396	28.888	31.35	20.404	1.00	27.02
1449	N	ARG	A	397	26.821	30.57	20.046	1.00	25.37
1450	CA	ARG	A	397	26.27	31.89	19.804	1.00	24.60
1451	CB	ARG	A	397	24.784	31.79	19.463	1.00	23.34
1452	CG	ARG	A	397	24.477	30.85	18.313	1.00	19.60
1453	CD	ARG	A	397	25.267	31.21	17.066	1.00	20.49
1454	NE	ARG	A	397	24.765	30.48	15.905	1.00	14.79
1455	CZ	ARG	A	397	25.326	30.5	14.703	1.00	16.61

1456	NH1	ARG	A	397	26.427	31.22	14.486	1.00	14.39
1457	NH2	ARG	A	397	24.786	29.8	13.717	1.00	14.57
1458	C	ARG	A	397	26.456	32.84	20.985	1.00	26.30
1459	O	ARG	A	397	26.283	32.45	22.14	1.00	26.77
1460	N	PRO	A	398	26.822	34.1	20.704	1.00	27.02
1461	CD	PRO	A	398	27.21	34.63	19.386	1.00	26.91
1462	CA	PRO	A	398	27.026	35.1	21.752	1.00	27.46
1463	CB	PRO	A	398	27.449	36.34	20.964	1.00	28.18
1464	CG	PRO	A	398	28.124	35.77	19.765	1.00	28.30
1465	C	PRO	A	398	25.735	35.35	22.534	1.00	28.08
1466	O	PRO	A	398	24.643	35.27	21.975	1.00	28.60
1467	N	GLY	A	399	25.872	35.63	23.826	1.00	27.99
1468	CA	GLY	A	399	24.716	35.92	24.66	1.00	27.31
1469	C	GLY	A	399	23.795	34.79	25.072	1.00	26.48
1470	O	GLY	A	399	22.714	35.04	25.603	1.00	25.44
1471	N	LEU	A	400	24.197	33.54	24.833	1.00	25.96
1472	CA	LEU	A	400	23.365	32.4	25.209	1.00	26.11
1473	CB	LEU	A	400	23.807	31.14	24.474	1.00	26.09
1474	CG	LEU	A	400	23.406	30.99	23.006	1.00	25.05
1475	CD1	LEU	A	400	24.037	29.73	22.44	1.00	23.61
1476	CD2	LEU	A	400	21.892	30.93	22.889	1.00	23.97
1477	C	LEU	A	400	23.431	32.14	26.706	1.00	27.86
1478	O	LEU	A	400	24.473	32.34	27.334	1.00	26.88
1479	N	LEU	A	401	22.318	31.67	27.261	1.00	28.14
1480	CA	LEU	A	401	22.233	31.38	28.684	1.00	31.00
1481	CB	LEU	A	401	20.865	31.8	29.228	1.00	30.68
1482	CG	LEU	A	401	20.578	31.45	30.691	1.00	32.59
1483	CD1	LEU	A	401	21.62	32.1	31.597	1.00	32.90
1484	CD2	LEU	A	401	19.179	31.92	31.06	1.00	31.69
1485	C	LEU	A	401	22.429	29.89	28.943	1.00	31.60
1486	O	LEU	A	401	23.369	29.48	29.622	1.00	33.05
1487	N	ASN	A	402	21.532	29.09	28.383	1.00	31.62
1488	CA	ASN	A	402	21.56	27.65	28.559	1.00	32.32
1489	CB	ASN	A	402	20.142	27.12	28.394	1.00	34.00

1490	CG	ASN	A	402	19.94	25.79	29.062	1.00	36.18
1491	OD1	ASN	A	402	18.817	25.3	29.135	1.00	38.80
1492	ND2	ASN	A	402	21.022	25.2	29.558	1.00	37.30
1493	C	ASN	A	402	22.508	26.95	27.584	1.00	31.82
1494	O	ASN	A	402	22.123	25.98	26.925	1.00	30.71
1495	N	VAL	A	403	23.746	27.42	27.514	1.00	31.16
1496	CA	VAL	A	403	24.752	26.85	26.624	1.00	31.48
1497	CB	VAL	A	403	26.143	27.48	26.903	1.00	31.26
1498	CG1	VAL	A	403	26.484	27.35	28.377	1.00	32.59
1499	CG2	VAL	A	403	27.211	26.82	26.045	1.00	31.72
1500	C	VAL	A	403	24.847	25.32	26.73	1.00	31.80
1501	O	VAL	A	403	24.987	24.63	25.72	1.00	32.39
1502	N	GLY	A	404	24.756	24.8	27.949	1.00	30.80
1503	CA	GLY	A	404	24.836	23.36	28.141	1.00	30.87
1504	C	GLY	A	404	23.746	22.57	27.442	1.00	31.11
1505	O	GLY	A	404	24.032	21.62	26.71	1.00	31.28
1506	N	HIS	A	405	22.493	22.95	27.661	1.00	30.39
1507	CA	HIS	A	405	21.37	22.26	27.051	1.00	30.64
1508	CB	HIS	A	405	20.045	22.78	27.623	1.00	33.97
1509	CG	HIS	A	405	19.876	22.51	29.09	1.00	38.64
1510	CD2	HIS	A	405	18.885	22.85	29.952	1.00	40.99
1511	ND1	HIS	A	405	20.82	21.84	29.836	1.00	39.58
1512	CE1	HIS	A	405	20.42	21.77	31.094	1.00	41.27
1513	NE2	HIS	A	405	19.25	22.38	31.191	1.00	41.61
1514	C	HIS	A	405	21.385	22.38	25.53	1.00	29.36
1515	O	HIS	A	405	20.963	21.47	24.827	1.00	28.36
1516	N	ILE	A	406	21.881	23.5	25.024	1.00	27.89
1517	CA	ILE	A	406	21.943	23.71	23.58	1.00	27.60
1518	CB	ILE	A	406	22.21	25.19	23.238	1.00	25.64
1519	CG2	ILE	A	406	22.473	25.36	21.741	1.00	25.46
1520	CG1	ILE	A	406	20.993	26.03	23.636	1.00	23.43
1521	CD1	ILE	A	406	21.23	27.53	23.575	1.00	23.81
1522	C	ILE	A	406	23.023	22.82	22.961	1.00	28.42
1523	O	ILE	A	406	22.848	22.3	21.86	1.00	28.52

1524	N	GLU	A	407	24.132	22.63	23.673	1.00	28.38
1525	CA	GLU	A	407	25.21	21.79	23.165	1.00	30.86
1526	CB	GLU	A	407	26.435	21.85	24.087	1.00	31.87
1527	CG	GLU	A	407	27.059	23.22	24.208	1.00	35.51
1528	CD	GLU	A	407	28.343	23.21	25.016	1.00	37.24
1529	OE1	GLU	A	407	28.346	22.62	26.121	1.00	38.47
1530	OE2	GLU	A	407	29.345	23.79	24.548	1.00	39.11
1531	C	GLU	A	407	24.754	20.34	23.033	1.00	30.96
1532	O	GLU	A	407	25.116	19.65	22.081	1.00	32.65
1533	N	LYS	A	408	23.959	19.87	23.991	1.00	31.74
1534	CA	LYS	A	408	23.47	18.49	23.962	1.00	32.12
1535	CB	LYS	A	408	22.748	18.16	25.275	1.00	34.57
1536	CG	LYS	A	408	21.294	18.6	25.333	1.00	37.40
1537	CD	LYS	A	408	20.363	17.48	24.898	1.00	39.89
1538	CE	LYS	A	408	19.082	18.02	24.279	1.00	40.38
1539	NZ	LYS	A	408	18.438	19.07	25.118	1.00	42.06
1540	C	LYS	A	408	22.527	18.33	22.771	1.00	30.88
1541	O	LYS	A	408	22.44	17.26	22.168	1.00	29.64
1542	N	MET	A	409	21.827	19.41	22.436	1.00	30.20
1543	CA	MET	A	409	20.907	19.4	21.304	1.00	30.04
1544	CB	MET	A	409	20.125	20.71	21.259	1.00	31.30
1545	CG	MET	A	409	18.627	20.56	21.382	1.00	34.42
1546	SD	MET	A	409	17.79	22.14	21.137	1.00	37.50
1547	CE	MET	A	409	17.603	22.66	22.784	1.00	35.32
1548	C	MET	A	409	21.703	19.25	20.01	1.00	28.14
1549	O	MET	A	409	21.397	18.4	19.172	1.00	27.06
1550	N	GLN	A	410	22.726	20.09	19.851	1.00	27.24
1551	CA	GLN	A	410	23.555	20.04	18.652	1.00	27.85
1552	CB	GLN	A	410	24.58	21.19	18.647	1.00	29.46
1553	CG	GLN	A	410	25.441	21.21	17.38	1.00	32.43
1554	CD	GLN	A	410	26.288	22.47	17.245	1.00	34.32
1555	OE1	GLN	A	410	27.097	22.79	18.115	1.00	34.44
1556	NE2	GLN	A	410	26.105	23.19	16.14	1.00	32.43
1557	C	GLN	A	410	24.275	18.71	18.545	1.00	27.48

1558	O	GLN	A	410	24.483	18.19	17.449	1.00	26.07
1559	N	GLU	A	411	24.645	18.14	19.691	1.00	27.34
1560	CA	GLU	A	411	25.339	16.86	19.731	1.00	28.25
1561	CB	GLU	A	411	25.621	16.46	21.186	1.00	30.37
1562	CG	GLU	A	411	26.281	15.09	21.341	1.00	35.80
1563	CD	GLU	A	411	26.58	14.74	22.791	1.00	38.57
1564	OE1	GLU	A	411	27.532	15.32	23.359	1.00	39.33
1565	OE2	GLU	A	411	25.858	13.89	23.364	1.00	39.79
1566	C	GLU	A	411	24.508	15.78	19.043	1.00	26.37
1567	O	GLU	A	411	25.022	15.03	18.213	1.00	26.12
1568	N	GLY	A	412	23.226	15.71	19.396	1.00	22.95
1569	CA	GLY	A	412	22.335	14.73	18.811	1.00	22.23
1570	C	GLY	A	412	22.12	14.94	17.323	1.00	22.14
1571	O	GLY	A	412	22.074	13.99	16.55	1.00	22.69
1572	N	ILE	A	413	21.984	16.2	16.918	1.00	20.27
1573	CA	ILE	A	413	21.785	16.53	15.507	1.00	20.28
1574	CB	ILE	A	413	21.5	18.06	15.334	1.00	18.92
1575	CG2	ILE	A	413	21.591	18.46	13.857	1.00	18.08
1576	CG1	ILE	A	413	20.124	18.38	15.919	1.00	20.64
1577	CD1	ILE	A	413	19.761	19.87	15.944	1.00	21.12
1578	C	ILE	A	413	23.01	16.13	14.686	1.00	20.45
1579	O	ILE	A	413	22.886	15.5	13.637	1.00	19.39
1580	N	VAL	A	414	24.191	16.49	15.177	1.00	22.04
1581	CA	VAL	A	414	25.438	16.16	14.493	1.00	24.01
1582	CB	VAL	A	414	26.648	16.76	15.237	1.00	24.63
1583	CG1	VAL	A	414	27.944	16.24	14.633	1.00	26.70
1584	CG2	VAL	A	414	26.604	18.28	15.152	1.00	25.08
1585	C	VAL	A	414	25.621	14.66	14.382	1.00	24.35
1586	O	VAL	A	414	26.059	14.15	13.352	1.00	24.50
1587	N	HIS	A	415	25.289	13.95	15.457	1.00	24.73
1588	CA	HIS	A	415	25.398	12.5	15.496	1.00	25.40
1589	CB	HIS	A	415	24.877	11.98	16.836	1.00	27.91
1590	CG	HIS	A	415	24.706	10.49	16.882	1.00	29.97
1591	CD2	HIS	A	415	23.603	9.718	16.752	1.00	31.72

1592	ND1	HIS	A	415	25.765	9.623	17.036	1.00	32.64
1593	CE1	HIS	A	415	25.321	8.379	16.999	1.00	31.24
1594	NE2	HIS	A	415	24.013	8.408	16.826	1.00	32.29
1595	C	HIS	A	415	24.576	11.89	14.363	1.00	24.78
1596	O	HIS	A	415	25.076	11.09	13.57	1.00	23.70
1597	N	VAL	A	416	23.308	12.29	14.302	1.00	24.16
1598	CA	VAL	A	416	22.393	11.8	13.28	1.00	24.60
1599	CB	VAL	A	416	20.96	12.32	13.548	1.00	26.47
1600	CG1	VAL	A	416	20.056	12.01	12.371	1.00	29.88
1601	CG2	VAL	A	416	20.411	11.66	14.809	1.00	27.86
1602	C	VAL	A	416	22.868	12.22	11.889	1.00	23.32
1603	O	VAL	A	416	22.743	11.46	10.927	1.00	21.28
1604	N	LEU	A	417	23.43	13.42	11.788	1.00	21.40
1605	CA	LEU	A	417	23.936	13.92	10.512	1.00	20.88
1606	CB	LEU	A	417	24.389	15.38	10.638	1.00	20.25
1607	CG	LEU	A	417	25.166	15.98	9.461	1.00	19.60
1608	CD1	LEU	A	417	24.323	15.92	8.189	1.00	18.77
1609	CD2	LEU	A	417	25.549	17.41	9.782	1.00	20.66
1610	C	LEU	A	417	25.103	13.06	10.031	1.00	21.76
1611	O	LEU	A	417	25.134	12.64	8.877	1.00	21.23
1612	N	ARG	A	418	26.056	12.78	10.921	1.00	22.31
1613	CA	ARG	A	418	27.214	11.97	10.551	1.00	23.13
1614	CB	ARG	A	418	28.166	11.78	11.738	1.00	25.75
1615	CG	ARG	A	418	29.481	11.11	11.325	1.00	30.84
1616	CD	ARG	A	418	30.375	10.73	12.502	1.00	34.64
1617	NE	ARG	A	418	30.554	11.83	13.446	1.00	36.72
1618	CZ	ARG	A	418	29.916	11.92	14.608	1.00	38.12
1619	NH1	ARG	A	418	29.061	10.98	14.969	1.00	40.03
1620	NH2	ARG	A	418	30.131	12.96	15.406	1.00	40.43
1621	C	ARG	A	418	26.795	10.6	10.036	1.00	23.39
1622	O	ARG	A	418	27.332	10.11	9.043	1.00	22.61
1623	N	LEU	A	419	25.837	9.988	10.721	1.00	22.60
1624	CA	LEU	A	419	25.35	8.67	10.333	1.00	24.37
1625	CB	LEU	A	419	24.453	8.101	11.439	1.00	24.59

1626	CG	LEU	A	419	25.209	7.675	12.708	1.00	27.68
1627	CD1	LEU	A	419	24.232	7.27	13.802	1.00	27.24
1628	CD2	LEU	A	419	26.141	6.522	12.37	1.00	26.90
1629	C	LEU	A	419	24.594	8.736	9.007	1.00	23.58
1630	O	LEU	A	419	24.753	7.87	8.141	1.00	22.71
1631	N	HIS	A	420	23.782	9.772	8.845	1.00	22.55
1632	CA	HIS	A	420	23.011	9.943	7.619	1.00	22.81
1633	CB	HIS	A	420	22.098	11.17	7.748	1.00	22.24
1634	CG	HIS	A	420	21.152	11.34	6.6	1.00	22.11
1635	CD2	HIS	A	420	19.934	10.8	6.361	1.00	23.05
1636	ND1	HIS	A	420	21.435	12.14	5.51	1.00	23.65
1637	CE1	HIS	A	420	20.435	12.08	4.649	1.00	20.84
1638	NE2	HIS	A	420	19.512	11.27	5.141	1.00	24.45
1639	C	HIS	A	420	23.929	10.09	6.407	1.00	22.74
1640	O	HIS	A	420	23.687	9.488	5.355	1.00	21.42
1641	N	LEU	A	421	24.985	10.89	6.553	1.00	20.60
1642	CA	LEU	A	421	25.926	11.09	5.458	1.00	22.09
1643	CB	LEU	A	421	26.967	12.15	5.837	1.00	21.12
1644	CG	LEU	A	421	26.44	13.58	6.022	1.00	20.72
1645	CD1	LEU	A	421	27.573	14.49	6.475	1.00	20.64
1646	CD2	LEU	A	421	25.832	14.07	4.708	1.00	21.54
1647	C	LEU	A	421	26.636	9.806	5.062	1.00	22.50
1648	O	LEU	A	421	26.916	9.584	3.885	1.00	22.76
1649	N	GLN	A	422	26.941	8.962	6.042	1.00	24.45
1650	CA	GLN	A	422	27.621	7.706	5.75	1.00	26.41
1651	CB	GLN	A	422	28.016	6.992	7.047	1.00	28.87
1652	CG	GLN	A	422	29.241	7.583	7.717	1.00	32.50
1653	CD	GLN	A	422	30.157	6.52	8.293	1.00	35.70
1654	OE1	GLN	A	422	29.819	5.852	9.27	1.00	36.19
1655	NE2	GLN	A	422	31.325	6.353	7.68	1.00	38.34
1656	C	GLN	A	422	26.765	6.781	4.888	1.00	26.96
1657	O	GLN	A	422	27.271	6.136	3.968	1.00	26.69
1658	N	SER	A	423	25.468	6.729	5.176	1.00	26.98
1659	CA	SER	A	423	24.555	5.88	4.417	1.00	27.71

1660	CB	SER	A	423	23.377	5.458	5.298	1.00	29.19
1661	OG	SER	A	423	22.558	6.566	5.623	1.00	33.45
1662	C	SER	A	423	24.02	6.524	3.137	1.00	26.94
1663	O	SER	A	423	23.724	5.825	2.17	1.00	27.54
1664	N	ASN	A	424	23.892	7.851	3.124	1.00	25.54
1665	CA	ASN	A	424	23.371	8.557	1.947	1.00	24.76
1666	CB	ASN	A	424	22.674	9.86	2.377	1.00	24.73
1667	CG	ASN	A	424	21.705	10.4	1.318	1.00	26.54
1668	OD1	ASN	A	424	21.319	11.57	1.348	1.00	25.37
1669	ND2	ASN	A	424	21.295	9.532	0.392	1.00	24.83
1670	C	ASN	A	424	24.468	8.873	0.928	1.00	24.23
1671	O	ASN	A	424	24.201	8.95	-0.271	1.00	23.51
1672	N	HIS	A	425	25.698	9.06	1.405	1.00	23.19
1673	CA	HIS	A	425	26.833	9.36	0.53	1.00	24.23
1674	CB	HIS	A	425	27.272	10.83	0.682	1.00	22.51
1675	CG	HIS	A	425	26.239	11.82	0.242	1.00	21.91
1676	CD2	HIS	A	425	26.002	12.38	-0.967	1.00	19.28
1677	ND1	HIS	A	425	25.284	12.33	1.096	1.00	22.80
1678	CE1	HIS	A	425	24.503	13.16	0.431	1.00	17.33
1679	NE2	HIS	A	425	24.917	13.21	-0.823	1.00	20.76
1680	C	HIS	A	425	28.016	8.451	0.862	1.00	26.11
1681	O	HIS	A	425	29.073	8.918	1.285	1.00	24.94
1682	N	PRO	A	426	27.856	7.136	0.65	1.00	29.11
1683	CD	PRO	A	426	26.708	6.467	0.008	1.00	29.49
1684	CA	PRO	A	426	28.922	6.174	0.94	1.00	30.85
1685	CB	PRO	A	426	28.248	4.831	0.67	1.00	31.26
1686	CG	PRO	A	426	27.321	5.157	-0.46	1.00	30.77
1687	C	PRO	A	426	30.193	6.361	0.119	1.00	33.62
1688	O	PRO	A	426	31.268	5.919	0.529	1.00	35.12
1689	N	ASP	A	427	30.08	7.013	-1.034	1.00	34.60
1690	CA	ASP	A	427	31.243	7.22	-1.883	1.00	36.67
1691	CB	ASP	A	427	30.827	7.268	-3.357	1.00	39.63
1692	CG	ASP	A	427	30.146	5.986	-3.814	1.00	41.06
1693	OD1	ASP	A	427	30.565	4.897	-3.366	1.00	42.57

1694	OD2	ASP	A	427	29.201	6.068	-4.629	1.00	43.11
1695	C	ASP	A	427	32.053	8.465	-1.542	1.00	37.42
1696	O	ASP	A	427	33.263	8.498	-1.774	1.00	37.62
1697	N	ASP	A	428	31.402	9.486	-0.99	1.00	37.02
1698	CA	ASP	A	428	32.126	10.71	-0.649	1.00	37.69
1699	CB	ASP	A	428	31.198	11.9	-0.46	1.00	36.87
1700	CG	ASP	A	428	31.972	13.21	-0.347	1.00	37.47
1701	OD1	ASP	A	428	33.072	13.21	0.248	1.00	36.42
1702	OD2	ASP	A	428	31.484	14.25	-0.847	1.00	37.98
1703	C	ASP	A	428	32.96	10.55	0.602	1.00	38.20
1704	O	ASP	A	428	32.451	10.39	1.714	1.00	37.99
1705	N	ILE	A	429	34.261	10.63	0.385	1.00	39.15
1706	CA	ILE	A	429	35.269	10.51	1.414	1.00	37.95
1707	CB	ILE	A	429	36.628	10.91	0.814	1.00	39.91
1708	CG2	ILE	A	429	37.047	9.889	-0.236	1.00	40.60
1709	CG1	ILE	A	429	36.508	12.29	0.139	1.00	41.10
1710	CD1	ILE	A	429	37.785	12.79	-0.515	1.00	42.96
1711	C	ILE	A	429	35.027	11.31	2.702	1.00	35.07
1712	O	ILE	A	429	34.534	10.78	3.698	1.00	35.43
1713	N	PHE	A	430	35.379	12.58	2.67	1.00	31.63
1714	CA	PHE	A	430	35.263	13.44	3.831	1.00	26.48
1715	CB	PHE	A	430	36.493	14.35	3.926	1.00	29.04
1716	CG	PHE	A	430	37.806	13.62	3.916	1.00	30.93
1717	CD1	PHE	A	430	38.349	13.15	2.729	1.00	33.42
1718	CD2	PHE	A	430	38.518	13.44	5.093	1.00	31.75
1719	CE1	PHE	A	430	39.592	12.51	2.714	1.00	34.29
1720	CE2	PHE	A	430	39.758	12.8	5.091	1.00	31.88
1721	CZ	PHE	A	430	40.296	12.34	3.9	1.00	33.09
1722	C	PHE	A	430	34.035	14.34	3.817	1.00	23.47
1723	O	PHE	A	430	34.15	15.51	4.167	1.00	21.09
1724	N	LEU	A	431	32.864	13.83	3.444	1.00	20.27
1725	CA	LEU	A	431	31.7	14.72	3.403	1.00	17.44
1726	CB	LEU	A	431	30.468	13.98	2.853	1.00	15.99
1727	CG	LEU	A	431	29.23	14.85	2.603	1.00	14.82

1728	CD1	LEU	A	431	29.603	16.1	1.815	1.00	15.78
1729	CD2	LEU	A	431	28.183	14.05	1.862	1.00	16.91
1730	C	LEU	A	431	31.378	15.38	4.747	1.00	17.17
1731	O	LEU	A	431	31	16.56	4.789	1.00	15.16
1732	N	PHE	A	432	31.533	14.65	5.852	1.00	15.85
1733	CA	PHE	A	432	31.243	15.25	7.156	1.00	15.61
1734	CB	PHE	A	432	31.332	14.19	8.267	1.00	17.14
1735	CG	PHE	A	432	30.971	14.71	9.629	1.00	18.64
1736	CD1	PHE	A	432	29.695	15.2	9.889	1.00	20.33
1737	CD2	PHE	A	432	31.906	14.71	10.657	1.00	20.31
1738	CE1	PHE	A	432	29.355	15.68	11.157	1.00	20.29
1739	CE2	PHE	A	432	31.576	15.18	11.93	1.00	21.44
1740	CZ	PHE	A	432	30.299	15.67	12.179	1.00	22.31
1741	C	PHE	A	432	32.196	16.41	7.451	1.00	16.28
1742	O	PHE	A	432	31.754	17.54	7.719	1.00	14.24
1743	N	PRO	A	433	33.52	16.17	7.422	1.00	17.45
1744	CD	PRO	A	433	34.282	14.91	7.339	1.00	17.91
1745	CA	PRO	A	433	34.396	17.31	7.704	1.00	16.84
1746	CB	PRO	A	433	35.796	16.68	7.766	1.00	19.13
1747	CG	PRO	A	433	35.663	15.4	6.995	1.00	18.96
1748	C	PRO	A	433	34.255	18.44	6.663	1.00	15.92
1749	O	PRO	A	433	34.466	19.61	6.974	1.00	15.44
1750	N	LYS	A	434	33.882	18.08	5.435	1.00	16.05
1751	CA	LYS	A	434	33.678	19.1	4.401	1.00	15.22
1752	CB	LYS	A	434	33.261	18.45	3.076	1.00	15.46
1753	CG	LYS	A	434	34.363	17.72	2.337	1.00	16.19
1754	CD	LYS	A	434	33.806	17.12	1.056	1.00	17.44
1755	CE	LYS	A	434	34.848	16.33	0.281	1.00	19.89
1756	NZ	LYS	A	434	34.259	15.78	-0.979	1.00	18.37
1757	C	LYS	A	434	32.561	20.03	4.857	1.00	14.66
1758	O	LYS	A	434	32.659	21.26	4.722	1.00	13.26
1759	N	LEU	A	435	31.495	19.45	5.397	1.00	13.97
1760	CA	LEU	A	435	30.351	20.22	5.869	1.00	14.01
1761	CB	LEU	A	435	29.154	19.31	6.134	1.00	14.60

1762	CG	LEU	A	435	28.489	18.73	4.885	1.00	18.11
1763	CD1	LEU	A	435	27.366	17.78	5.291	1.00	19.14
1764	CD2	LEU	A	435	27.947	19.86	4.019	1.00	19.11
1765	C	LEU	A	435	30.695	21.02	7.118	1.00	15.51
1766	O	LEU	A	435	30.2	22.14	7.303	1.00	16.69
1767	N	LEU	A	436	31.546	20.47	7.977	1.00	16.13
1768	CA	LEU	A	436	31.947	21.22	9.163	1.00	17.20
1769	CB	LEU	A	436	32.875	20.39	10.053	1.00	19.20
1770	CG	LEU	A	436	32.224	19.18	10.73	1.00	21.00
1771	CD1	LEU	A	436	33.252	18.44	11.581	1.00	22.86
1772	CD2	LEU	A	436	31.057	19.64	11.589	1.00	22.35
1773	C	LEU	A	436	32.667	22.47	8.693	1.00	17.44
1774	O	LEU	A	436	32.488	23.55	9.265	1.00	15.95
1775	N	GLN	A	437	33.481	22.35	7.647	1.00	16.16
1776	CA	GLN	A	437	34.183	23.53	7.137	1.00	16.84
1777	CB	GLN	A	437	35.235	23.15	6.09	1.00	17.05
1778	CG	GLN	A	437	36.012	24.37	5.576	1.00	20.71
1779	CD	GLN	A	437	36.985	24.04	4.46	1.00	22.77
1780	OE1	GLN	A	437	36.622	23.4	3.475	1.00	25.06
1781	NE2	GLN	A	437	38.227	24.5	4.604	1.00	26.03
1782	C	GLN	A	437	33.179	24.51	6.529	1.00	17.18
1783	O	GLN	A	437	33.329	25.72	6.668	1.00	17.33
1784	N	LYS	A	438	32.15	23.99	5.858	1.00	17.54
1785	CA	LYS	A	438	31.136	24.87	5.262	1.00	17.07
1786	CB	LYS	A	438	30.083	24.06	4.502	1.00	17.70
1787	CG	LYS	A	438	30.623	23.31	3.309	1.00	19.51
1788	CD	LYS	A	438	31.345	24.23	2.341	1.00	22.06
1789	CE	LYS	A	438	31.902	23.44	1.155	1.00	22.64
1790	NZ	LYS	A	438	32.819	24.28	0.343	1.00	21.64
1791	C	LYS	A	438	30.443	25.7	6.329	1.00	18.54
1792	O	LYS	A	438	30.07	26.85	6.084	1.00	16.97
1793	N	MET	A	439	30.257	25.12	7.512	1.00	18.74
1794	CA	MET	A	439	29.619	25.85	8.599	1.00	19.35
1795	CB	MET	A	439	29.426	24.95	9.814	1.00	22.86

1796	CG	MET	A	439	28.564	23.73	9.519	1.00	25.60
1797	SD	MET	A	439	28.191	22.76	10.972	1.00	29.86
1798	CE	MET	A	439	26.648	23.51	11.476	1.00	30.44
1799	C	MET	A	439	30.503	27.04	8.97	1.00	19.48
1800	O	MET	A	439	30.009	28.13	9.217	1.00	17.93
1801	N	ALA	A	440	31.815	26.82	9.007	1.00	19.56
1802	CA	ALA	A	440	32.762	27.88	9.34	1.00	18.57
1803	CB	ALA	A	440	34.153	27.29	9.549	1.00	20.87
1804	C	ALA	A	440	32.796	28.93	8.232	1.00	19.19
1805	O	ALA	A	440	32.903	30.13	8.496	1.00	18.72
1806	N	ASP	A	441	32.713	28.47	6.987	1.00	17.33
1807	CA	ASP	A	441	32.722	29.38	5.848	1.00	17.47
1808	CB	ASP	A	441	32.749	28.6	4.533	1.00	18.81
1809	CG	ASP	A	441	34.084	27.92	4.279	1.00	22.11
1810	OD1	ASP	A	441	35.081	28.28	4.93	1.00	23.74
1811	OD2	ASP	A	441	34.135	27.02	3.409	1.00	23.76
1812	C	ASP	A	441	31.479	30.26	5.888	1.00	17.16
1813	O	ASP	A	441	31.543	31.45	5.56	1.00	16.05
1814	N	LEU	A	442	30.351	29.69	6.299	1.00	15.92
1815	CA	LEU	A	442	29.1	30.44	6.373	1.00	15.51
1816	CB	LEU	A	442	27.921	29.5	6.648	1.00	14.97
1817	CG	LEU	A	442	27.461	28.65	5.457	1.00	16.25
1818	CD1	LEU	A	442	26.459	27.62	5.923	1.00	15.43
1819	CD2	LEU	A	442	26.835	29.54	4.389	1.00	16.30
1820	C	LEU	A	442	29.149	31.53	7.441	1.00	16.51
1821	O	LEU	A	442	28.64	32.62	7.243	1.00	15.91
1822	N	ARG	A	443	29.758	31.21	8.578	1.00	17.51
1823	CA	ARG	A	443	29.859	32.19	9.656	1.00	19.49
1824	CB	ARG	A	443	30.545	31.56	10.868	1.00	20.19
1825	CG	ARG	A	443	30.518	32.44	12.104	1.00	24.32
1826	CD	ARG	A	443	30.919	31.66	13.334	1.00	27.77
1827	NE	ARG	A	443	29.938	30.63	13.68	1.00	30.42
1828	CZ	ARG	A	443	29.983	29.92	14.799	1.00	32.49
1829	NH1	ARG	A	443	30.963	30.12	15.669	1.00	33.93

1830	NH2	ARG	A	443	29.052	29.01	15.058	1.00	32.62
1831	C	ARG	A	443	30.649	33.4	9.171	1.00	19.24
1832	O	ARG	A	443	30.288	34.54	9.451	1.00	20.11
1833	N	GLN	A	444	31.729	33.15	8.441	1.00	20.35
1834	CA	GLN	A	444	32.555	34.23	7.906	1.00	21.41
1835	CB	GLN	A	444	33.831	33.66	7.278	1.00	23.62
1836	CG	GLN	A	444	34.618	34.65	6.433	1.00	28.57
1837	CD	GLN	A	444	35.508	35.57	7.25	1.00	33.29
1838	OE1	GLN	A	444	35.105	36.09	8.293	1.00	36.07
1839	NE2	GLN	A	444	36.728	35.79	6.768	1.00	36.08
1840	C	GLN	A	444	31.761	34.99	6.852	1.00	20.82
1841	O	GLN	A	444	31.776	36.22	6.815	1.00	19.43
1842	N	LEU	A	445	31.062	34.25	5.997	1.00	19.72
1843	CA	LEU	A	445	30.255	34.85	4.943	1.00	18.86
1844	CB	LEU	A	445	29.577	33.75	4.112	1.00	18.95
1845	CG	LEU	A	445	28.856	34.16	2.826	1.00	20.08
1846	CD1	LEU	A	445	29.888	34.62	1.793	1.00	20.86
1847	CD2	LEU	A	445	28.06	32.97	2.275	1.00	21.90
1848	C	LEU	A	445	29.19	35.78	5.53	1.00	18.74
1849	O	LEU	A	445	28.909	36.84	4.963	1.00	17.29
1850	N	VAL	A	446	28.596	35.39	6.658	1.00	17.24
1851	CA	VAL	A	446	27.565	36.23	7.287	1.00	17.47
1852	CB	VAL	A	446	26.781	35.45	8.367	1.00	17.76
1853	CG1	VAL	A	446	25.852	36.4	9.126	1.00	18.67
1854	CG2	VAL	A	446	25.955	34.34	7.711	1.00	14.52
1855	C	VAL	A	446	28.171	37.48	7.927	1.00	18.46
1856	O	VAL	A	446	27.612	38.57	7.832	1.00	18.68
1857	N	THR	A	447	29.311	37.3	8.584	1.00	18.45
1858	CA	THR	A	447	29.984	38.42	9.232	1.00	19.82
1859	CB	THR	A	447	31.313	37.97	9.872	1.00	20.76
1860	OG1	THR	A	447	31.048	36.96	10.85	1.00	22.73
1861	CG2	THR	A	447	32.008	39.14	10.542	1.00	23.28
1862	C	THR	A	447	30.272	39.5	8.197	1.00	20.08
1863	O	THR	A	447	30.04	40.69	8.434	1.00	20.49

1864	N	GLU	A	448	30.777	39.07	7.044	1.00	18.53
1865	CA	GLU	A	448	31.104	39.98	5.963	1.00	19.18
1866	CB	GLU	A	448	31.901	39.23	4.889	1.00	19.51
1867	CG	GLU	A	448	33.064	38.45	5.485	1.00	23.78
1868	CD	GLU	A	448	33.905	37.72	4.454	1.00	25.56
1869	OE1	GLU	A	448	33.331	37.13	3.518	1.00	27.66
1870	OE2	GLU	A	448	35.147	37.73	4.592	1.00	27.05
1871	C	GLU	A	448	29.85	40.61	5.358	1.00	17.55
1872	O	GLU	A	448	29.86	41.77	4.961	1.00	18.18
1873	N	HIS	A	449	28.771	39.84	5.283	1.00	16.47
1874	CA	HIS	A	449	27.526	40.35	4.729	1.00	15.35
1875	CB	HIS	A	449	26.509	39.22	4.559	1.00	13.45
1876	CG	HIS	A	449	25.167	39.67	4.061	1.00	13.44
1877	CD2	HIS	A	449	24	39.87	4.715	1.00	14.46
1878	ND1	HIS	A	449	24.914	39.94	2.734	1.00	14.54
1879	CE1	HIS	A	449	23.65	40.3	2.593	1.00	14.39
1880	NE2	HIS	A	449	23.072	40.26	3.78	1.00	14.22
1881	C	HIS	A	449	26.949	41.44	5.633	1.00	15.34
1882	O	HIS	A	449	26.508	42.48	5.145	1.00	16.88
1883	N	ALA	A	450	26.953	41.22	6.942	1.00	16.12
1884	CA	ALA	A	450	26.422	42.2	7.883	1.00	17.96
1885	CB	ALA	A	450	26.507	41.67	9.31	1.00	17.75
1886	C	ALA	A	450	27.191	43.52	7.776	1.00	19.46
1887	O	ALA	A	450	26.623	44.6	7.958	1.00	18.94
1888	N	GLN	A	451	28.482	43.43	7.481	1.00	21.32
1889	CA	GLN	A	451	29.31	44.63	7.348	1.00	22.42
1890	CB	GLN	A	451	30.779	44.25	7.151	1.00	26.37
1891	CG	GLN	A	451	31.721	45.44	7.069	1.00	31.72
1892	CD	GLN	A	451	33.179	45.03	6.974	1.00	34.48
1893	OE1	GLN	A	451	33.653	44.21	7.757	1.00	37.93
1894	NE2	GLN	A	451	33.897	45.6	6.016	1.00	35.81
1895	C	GLN	A	451	28.831	45.45	6.161	1.00	21.76
1896	O	GLN	A	451	28.707	46.67	6.247	1.00	20.34
1897	N	LEU	A	452	28.556	44.77	5.05	1.00	19.43

1898	CA	LEU	A	452	28.086	45.46	3.855	1.00	20.58
1899	CB	LEU	A	452	28.063	44.5	2.662	1.00	21.26
1900	CG	LEU	A	452	27.566	45.09	1.338	1.00	23.72
1901	CD1	LEU	A	452	28.481	46.24	0.906	1.00	23.27
1902	CD2	LEU	A	452	27.531	44	0.277	1.00	23.43
1903	C	LEU	A	452	26.688	46.01	4.107	1.00	19.34
1904	O	LEU	A	452	26.369	47.12	3.676	1.00	20.88
1905	N	VAL	A	453	25.857	45.25	4.811	1.00	19.86
1906	CA	VAL	A	453	24.501	45.69	5.125	1.00	19.89
1907	CB	VAL	A	453	23.719	44.61	5.923	1.00	21.23
1908	CG1	VAL	A	453	22.35	45.14	6.342	1.00	22.52
1909	CG2	VAL	A	453	23.538	43.36	5.063	1.00	20.41
1910	C	VAL	A	453	24.557	46.99	5.938	1.00	21.15
1911	O	VAL	A	453	23.745	47.89	5.733	1.00	20.95
1912	N	GLN	A	454	25.522	47.08	6.847	1.00	21.46
1913	CA	GLN	A	454	25.669	48.28	7.667	1.00	23.89
1914	CB	GLN	A	454	26.729	48.05	8.749	1.00	27.62
1915	CG	GLN	A	454	26.848	49.2	9.754	1.00	32.28
1916	CD	GLN	A	454	25.615	49.35	10.635	1.00	35.43
1917	OE1	GLN	A	454	25.592	50.18	11.546	1.00	38.17
1918	NE2	GLN	A	454	24.586	48.55	10.371	1.00	37.92
1919	C	GLN	A	454	26.066	49.47	6.789	1.00	24.56
1920	O	GLN	A	454	25.59	50.58	6.993	1.00	22.97
1921	N	ILE	A	455	26.938	49.22	5.817	1.00	23.13
1922	CA	ILE	A	455	27.383	50.27	4.915	1.00	24.75
1923	CB	ILE	A	455	28.474	49.75	3.948	1.00	24.82
1924	CG2	ILE	A	455	28.746	50.76	2.846	1.00	24.01
1925	CG1	ILE	A	455	29.755	49.45	4.738	1.00	25.40
1926	CD1	ILE	A	455	30.846	48.78	3.935	1.00	25.53
1927	C	ILE	A	455	26.203	50.79	4.109	1.00	25.90
1928	O	ILE	A	455	26	52	3.969	1.00	26.44
1929	N	ILE	A	456	25.41	49.86	3.578	1.00	26.77
1930	CA	ILE	A	456	24.232	50.2	2.798	1.00	29.88
1931	CB	ILE	A	456	23.559	48.93	2.21	1.00	30.75

1932	CG2	ILE	A	456	22.188	49.27	1.69	1.00	33.39
1933	CG1	ILE	A	456	24.366	48.35	1.059	1.00	31.69
1934	CD1	ILE	A	456	23.79	47.03	0.547	1.00	34.09
1935	C	ILE	A	456	23.244	50.94	3.689	1.00	30.49
1936	O	ILE	A	456	22.611	51.92	3.278	1.00	30.43
1937	N	LYS	A	457	23.101	50.5	4.922	1.00	32.72
1938	CA	LYS	A	457	22.172	51.15	5.818	1.00	36.04
1939	CB	LYS	A	457	22.139	50.37	7.131	1.00	37.66
1940	CG	LYS	A	457	21.215	50.95	8.145	1.00	40.69
1941	CD	LYS	A	457	20.92	49.91	9.19	1.00	41.72
1942	CE	LYS	A	457	19.917	50.43	10.191	1.00	44.25
1943	NZ	LYS	A	457	20.495	51.43	11.136	1.00	45.65
1944	C	LYS	A	457	22.479	52.63	6.094	1.00	36.68
1945	O	LYS	A	457	21.564	53.45	6.176	1.00	36.26
1946	N	LYS	A	458	23.756	52.97	6.213	1.00	37.99
1947	CA	LYS	A	458	24.132	54.35	6.501	1.00	39.24
1948	CB	LYS	A	458	25.327	54.38	7.465	1.00	41.14
1949	CG	LYS	A	458	26.689	54.41	6.785	1.00	43.28
1950	CD	LYS	A	458	27.822	54.42	7.806	1.00	44.36
1951	CE	LYS	A	458	27.936	53.09	8.516	1.00	45.26
1952	NZ	LYS	A	458	28.212	51.99	7.55	1.00	44.67
1953	C	LYS	A	458	24.459	55.18	5.258	1.00	39.55
1954	O	LYS	A	458	24.528	56.41	5.321	1.00	39.79
1955	N	THR	A	459	24.65	54.5	4.132	1.00	39.02
1956	CA	THR	A	459	24.988	55.16	2.88	1.00	39.78
1957	CB	THR	A	459	26.164	54.43	2.182	1.00	40.83
1958	OG1	THR	A	459	27.404	54.92	2.715	1.00	41.96
1959	CG2	THR	A	459	26.136	54.65	0.68	1.00	42.44
1960	C	THR	A	459	23.823	55.29	1.901	1.00	39.33
1961	O	THR	A	459	23.734	56.27	1.16	1.00	39.15
1962	N	GLU	A	460	22.934	54.31	1.892	1.00	38.93
1963	CA	GLU	A	460	21.792	54.33	0.989	1.00	39.36
1964	CB	GLU	A	460	21.621	52.97	0.312	1.00	37.13
1965	CG	GLU	A	460	22.799	52.51	-0.549	1.00	33.20

1966	CD	GLU	A	460	22.988	53.33	-1.812	1.00	31.38
1967	OE1	GLU	A	460	21.988	53.86	-2.345	1.00	31.23
1968	OE2	GLU	A	460	24.137	53.44	-2.288	1.00	27.05
1969	C	GLU	A	460	20.514	54.69	1.742	1.00	41.61
1970	O	GLU	A	460	19.856	53.82	2.308	1.00	41.95
1971	N	SER	A	461	20.167	55.97	1.755	1.00	44.12
1972	CA	SER	A	461	18.958	56.41	2.439	1.00	46.91
1973	CB	SER	A	461	19.07	57.89	2.821	1.00	47.79
1974	OG	SER	A	461	20.075	58.09	3.805	1.00	49.02
1975	C	SER	A	461	17.769	56.2	1.516	1.00	48.12
1976	O	SER	A	461	16.613	56.29	1.928	1.00	48.49
1977	N	ASP	A	462	18.077	55.91	0.257	1.00	49.25
1978	CA	ASP	A	462	17.068	55.65	-0.758	1.00	50.01
1979	CB	ASP	A	462	17.751	55.26	-2.067	1.00	51.19
1980	CG	ASP	A	462	19.027	54.46	-1.839	1.00	51.21
1981	OD1	ASP	A	462	19.959	55.01	-1.215	1.00	52.21
1982	OD2	ASP	A	462	19.103	53.3	-2.279	1.00	52.20
1983	C	ASP	A	462	16.161	54.53	-0.285	1.00	49.54
1984	O	ASP	A	462	14.948	54.57	-0.482	1.00	50.36
1985	N	ALA	A	463	16.769	53.54	0.346	1.00	49.32
1986	CA	ALA	A	463	16.044	52.39	0.864	1.00	47.69
1987	CB	ALA	A	463	16.147	51.24	-0.105	1.00	48.66
1988	C	ALA	A	463	16.65	52.01	2.209	1.00	46.49
1989	O	ALA	A	463	17.867	52.01	2.365	1.00	47.87
1990	N	ALA	A	464	15.797	51.69	3.177	1.00	43.89
1991	CA	ALA	A	464	16.251	51.34	4.514	1.00	41.22
1992	CB	ALA	A	464	15.312	51.94	5.553	1.00	41.01
1993	C	ALA	A	464	16.349	49.83	4.714	1.00	39.82
1994	O	ALA	A	464	17.077	49.14	3.987	1.00	41.52
1995	N	LEU	A	465	15.628	49.33	5.715	1.00	36.01
1996	CA	LEU	A	465	15.588	47.9	6.058	1.00	32.30
1997	CB	LEU	A	465	16.754	47.51	6.977	1.00	33.09
1998	CG	LEU	A	465	18.085	47.02	6.399	1.00	33.05
1999	CD1	LEU	A	465	18.95	46.51	7.545	1.00	32.55

2000	CD2	LEU	A	465	17.854	45.9	5.398	1.00	31.55
2001	C	LEU	A	465	14.284	47.56	6.771	1.00	29.76
2002	O	LEU	A	465	13.78	48.34	7.59	1.00	26.72
2003	N	HIS	A	466	13.749	46.38	6.458	1.00	26.87
2004	CA	HIS	A	466	12.511	45.9	7.057	1.00	25.80
2005	CB	HIS	A	466	12.115	44.56	6.418	1.00	24.73
2006	CG	HIS	A	466	10.849	43.98	6.964	1.00	25.28
2007	CD2	HIS	A	466	10.576	43.4	8.157	1.00	24.58
2008	ND1	HIS	A	466	9.678	43.92	6.237	1.00	26.52
2009	CE1	HIS	A	466	8.739	43.34	6.959	1.00	25.66
2010	NE2	HIS	A	466	9.259	43.01	8.13	1.00	26.42
2011	C	HIS	A	466	12.716	45.72	8.563	1.00	25.90
2012	O	HIS	A	466	13.796	45.33	9.009	1.00	25.20
2013	N	PRO	A	467	11.674	46	9.364	1.00	25.60
2014	CD	PRO	A	467	10.372	46.55	8.935	1.00	26.08
2015	CA	PRO	A	467	11.724	45.87	10.823	1.00	25.42
2016	CB	PRO	A	467	10.262	46.04	11.223	1.00	25.91
2017	CG	PRO	A	467	9.78	47.04	10.238	1.00	27.38
2018	C	PRO	A	467	12.317	44.56	11.335	1.00	25.07
2019	O	PRO	A	467	13.16	44.56	12.233	1.00	25.29
2020	N	LEU	A	468	11.873	43.44	10.774	1.00	23.71
2021	CA	LEU	A	468	12.378	42.15	11.215	1.00	22.76
2022	CB	LEU	A	468	11.611	41	10.538	1.00	22.31
2023	CG	LEU	A	468	12.092	39.58	10.878	1.00	22.34
2024	CD1	LEU	A	468	11.953	39.32	12.379	1.00	23.76
2025	CD2	LEU	A	468	11.277	38.57	10.09	1.00	22.76
2026	C	LEU	A	468	13.866	42	10.927	1.00	22.18
2027	O	LEU	A	468	14.617	41.49	11.756	1.00	21.97
2028	N	LEU	A	469	14.296	42.44	9.752	1.00	21.66
2029	CA	LEU	A	469	15.704	42.34	9.394	1.00	21.60
2030	CB	LEU	A	469	15.885	42.62	7.899	1.00	20.70
2031	CG	LEU	A	469	14.968	41.76	7.024	1.00	19.18
2032	CD1	LEU	A	469	15.329	41.95	5.56	1.00	20.00
2033	CD2	LEU	A	469	15.104	40.29	7.424	1.00	16.85

2034	C	LEU	A	469	16.534	43.3	10.231	1.00	23.25
2035	O	LEU	A	469	17.671	43.01	10.613	1.00	21.71
2036	N	GLN	A	470	15.953	44.46	10.531	1.00	23.59
2037	CA	GLN	A	470	16.649	45.44	11.332	1.00	26.43
2038	CB	GLN	A	470	15.819	46.72	11.436	1.00	28.61
2039	CG	GLN	A	470	16.52	47.84	12.192	1.00	34.25
2040	CD	GLN	A	470	17.805	48.3	11.52	1.00	36.90
2041	OE1	GLN	A	470	18.567	49.08	12.092	1.00	40.50
2042	NE2	GLN	A	470	18.048	47.82	10.303	1.00	38.17
2043	C	GLN	A	470	16.95	44.9	12.727	1.00	25.75
2044	O	GLN	A	470	18.057	45.07	13.229	1.00	27.57
2045	N	GLU	A	471	15.986	44.22	13.354	1.00	25.39
2046	CA	GLU	A	471	16.239	43.7	14.693	1.00	26.81
2047	CB	GLU	A	471	14.929	43.29	15.397	1.00	28.93
2048	CG	GLU	A	471	14.136	42.15	14.784	1.00	30.21
2049	CD	GLU	A	471	12.837	41.88	15.551	1.00	32.16
2050	OE1	GLU	A	471	11.987	42.79	15.629	1.00	32.22
2051	OE2	GLU	A	471	12.665	40.76	16.077	1.00	30.73
2052	C	GLU	A	471	17.24	42.55	14.681	1.00	25.84
2053	O	GLU	A	471	17.978	42.34	15.648	1.00	25.91
2054	N	ILE	A	472	17.287	41.79	13.586	1.00	23.23
2055	CA	ILE	A	472	18.238	40.7	13.498	1.00	22.62
2056	CB	ILE	A	472	17.941	39.78	12.282	1.00	23.65
2057	CG2	ILE	A	472	19.106	38.81	12.049	1.00	21.96
2058	CG1	ILE	A	472	16.642	39.01	12.531	1.00	22.25
2059	CD1	ILE	A	472	16.172	38.18	11.345	1.00	24.20
2060	C	ILE	A	472	19.656	41.27	13.392	1.00	23.04
2061	O	ILE	A	472	20.567	40.79	14.061	1.00	20.73
2062	N	TYR	A	473	19.836	42.3	12.57	1.00	23.82
2063	CA	TYR	A	473	21.159	42.9	12.394	1.00	25.85
2064	CB	TYR	A	473	21.233	43.63	11.057	1.00	24.50
2065	CG	TYR	A	473	21.41	42.69	9.887	1.00	22.75
2066	CD1	TYR	A	473	22.574	41.94	9.749	1.00	23.07
2067	CE1	TYR	A	473	22.723	41.03	8.695	1.00	22.58

2068	CD2	TYR	A	473	20.401	42.53	8.945	1.00	23.44
2069	CE2	TYR	A	473	20.539	41.63	7.896	1.00	20.95
2070	CZ	TYR	A	473	21.698	40.89	7.777	1.00	22.05
2071	OH	TYR	A	473	21.822	39.99	6.74	1.00	21.31
2072	C	TYR	A	473	21.608	43.82	13.519	1.00	27.80
2073	O	TYR	A	473	22.805	44.05	13.69	1.00	28.04
2074	N	ARG	A	474	20.661	44.36	14.282	1.00	29.91
2075	CA	ARG	A	474	21.006	45.25	15.391	1.00	33.29
2076	CB	ARG	A	474	19.737	45.78	16.068	1.00	35.76
2077	CG	ARG	A	474	19.987	46.55	17.366	1.00	38.99
2078	CD	ARG	A	474	18.675	47.02	17.984	1.00	42.46
2079	NE	ARG	A	474	18.862	47.7	19.265	1.00	44.44
2080	CZ	ARG	A	474	17.879	48.28	19.953	1.00	46.85
2081	NH1	ARG	A	474	16.637	48.26	19.485	1.00	47.83
2082	NH2	ARG	A	474	18.134	48.87	21.111	1.00	47.38
2083	C	ARG	A	474	21.859	44.51	16.42	1.00	34.75
2084	O	ARG	A	474	21.409	43.53	17.025	1.00	34.47
2085	N	ASP	A	475	23.094	44.97	16.604	1.00	36.62
2086	CA	ASP	A	475	24.019	44.37	17.563	1.00	38.83
2087	CB	ASP	A	475	23.447	44.45	18.982	1.00	39.46
2088	CG	ASP	A	475	23.228	45.88	19.434	1.00	40.61
2089	OD1	ASP	A	475	24.135	46.72	19.217	1.00	40.51
2090	OD2	ASP	A	475	22.156	46.17	20.014	1.00	40.94
2091	C	ASP	A	475	24.396	42.92	17.274	1.00	39.96
2092	O	ASP	A	475	24.768	42.18	18.187	1.00	39.85
2093	N	MET	A	476	24.303	42.5	16.015	1.00	41.66
2094	CA	MET	A	476	24.664	41.13	15.66	1.00	43.69
2095	CB	MET	A	476	24.33	40.85	14.196	1.00	43.01
2096	CG	MET	A	476	24.632	39.42	13.777	1.00	43.53
2097	SD	MET	A	476	24.318	39.13	12.035	1.00	45.18
2098	CE	MET	A	476	22.532	38.88	12.057	1.00	44.23
2099	C	MET	A	476	26.163	40.97	15.882	1.00	45.56
2100	O	MET	A	476	26.603	40.18	16.718	1.00	46.26
2101	N	TYR	A	477	26.942	41.73	15.12	1.00	46.99

2102	CA	TYR	A	477	28.394	41.7	15.225	1.00	48.84
2103	CB	TYR	A	477	29.023	41.13	13.949	1.00	48.71
2104	CG	TYR	A	477	28.735	39.65	13.725	1.00	48.95
2105	CD1	TYR	A	477	27.925	39.23	12.67	1.00	49.23
2106	CE1	TYR	A	477	27.653	37.88	12.466	1.00	49.07
2107	CD2	TYR	A	477	29.268	38.68	14.574	1.00	49.57
2108	CE2	TYR	A	477	29.003	37.33	14.381	1.00	49.37
2109	CZ	TYR	A	477	28.196	36.93	13.327	1.00	49.98
2110	OH	TYR	A	477	27.937	35.59	13.14	1.00	49.98
2111	C	TYR	A	477	28.888	43.13	15.459	1.00	49.62
2112	O	TYR	A	477	29.046	43.86	14.465	1.00	50.21
2113	OT	TYR	A	477	29.08	43.5	16.638	1.00	50.66
2114	CB	GLU	B	685	18.563	43.31	21.966	1.00	63.65
2115	CG	GLU	B	685	18.355	43.18	23.466	1.00	63.87
2116	CD	GLU	B	685	18.5	41.75	23.944	1.00	64.23
2117	OE1	GLU	B	685	17.602	40.93	23.645	1.00	64.28
2118	OE2	GLU	B	685	19.509	41.44	24.611	1.00	64.53
2119	C	GLU	B	685	16.485	44.44	21.146	1.00	61.94
2120	O	GLU	B	685	15.976	44.7	20.055	1.00	62.27
2121	N	GLU	B	685	18.315	45.76	22.219	1.00	62.90
2122	CA	GLU	B	685	17.989	44.59	21.355	1.00	62.73
2123	N	ARG	B	686	15.783	44.01	22.191	1.00	60.58
2124	CA	ARG	B	686	14.335	43.82	22.134	1.00	59.13
2125	CB	ARG	B	686	13.674	45.08	21.56	1.00	60.07
2126	CG	ARG	B	686	12.151	45.06	21.524	1.00	61.27
2127	CD	ARG	B	686	11.543	45.61	22.805	1.00	62.16
2128	NE	ARG	B	686	10.168	46.05	22.594	1.00	63.43
2129	CZ	ARG	B	686	9.147	45.24	22.329	1.00	64.44
2130	NH1	ARG	B	686	9.339	43.93	22.247	1.00	64.89
2131	NH2	ARG	B	686	7.936	45.75	22.128	1.00	65.34
2132	C	ARG	B	686	13.932	42.6	21.299	1.00	57.39
2133	O	ARG	B	686	13.69	41.52	21.841	1.00	58.48
2134	N	HIS	B	687	13.867	42.78	19.982	1.00	54.71
2135	CA	HIS	B	687	13.479	41.72	19.052	1.00	51.16

2136	CB	HIS	B	687	14.316	40.46	19.28	1.00	51.72
2137	CG	HIS	B	687	15.776	40.64	19.004	1.00	51.47
2138	CD2	HIS	B	687	16.561	40.16	18.01	1.00	51.61
2139	ND1	HIS	B	687	16.596	41.41	19.802	1.00	52.04
2140	CE1	HIS	B	687	17.822	41.39	19.311	1.00	51.83
2141	NE2	HIS	B	687	17.828	40.64	18.225	1.00	51.34
2142	C	HIS	B	687	11.998	41.39	19.21	1.00	48.80
2143	O	HIS	B	687	11.628	40.24	19.412	1.00	48.44
2144	N	ALA	B	688	11.157	42.41	19.108	1.00	45.79
2145	CA	ALA	B	688	9.714	42.25	19.251	1.00	43.75
2146	CB	ALA	B	688	9.027	43.61	19.108	1.00	43.70
2147	C	ALA	B	688	9.106	41.26	18.265	1.00	41.94
2148	O	ALA	B	688	8.488	40.27	18.669	1.00	40.94
2149	N	ILE	B	689	9.282	41.52	16.973	1.00	40.75
2150	CA	ILE	B	689	8.728	40.65	15.939	1.00	39.42
2151	CB	ILE	B	689	9.093	41.17	14.532	1.00	39.12
2152	CG2	ILE	B	689	8.624	40.18	13.468	1.00	38.63
2153	CG1	ILE	B	689	8.444	42.54	14.312	1.00	38.90
2154	CD1	ILE	B	689	8.728	43.15	12.959	1.00	39.20
2155	C	ILE	B	689	9.18	39.2	16.077	1.00	38.83
2156	O	ILE	B	689	8.36	38.28	16.039	1.00	37.60
2157	N	LEU	B	690	10.482	39	16.24	1.00	38.40
2158	CA	LEU	B	690	11.027	37.66	16.389	1.00	38.63
2159	CB	LEU	B	690	12.54	37.74	16.596	1.00	39.36
2160	CG	LEU	B	690	13.378	36.57	16.066	1.00	40.30
2161	CD1	LEU	B	690	14.853	36.95	16.107	1.00	39.81
2162	CD2	LEU	B	690	13.111	35.32	16.884	1.00	41.50
2163	C	LEU	B	690	10.352	36.99	17.584	1.00	39.78
2164	O	LEU	B	690	9.892	35.85	17.491	1.00	38.83
2165	N	HIS	B	691	10.287	37.7	18.707	1.00	40.27
2166	CA	HIS	B	691	9.64	37.17	19.902	1.00	41.72
2167	CB	HIS	B	691	9.659	38.2	21.029	1.00	43.49
2168	CG	HIS	B	691	10.89	38.15	21.877	1.00	45.34
2169	CD2	HIS	B	691	11.897	39.04	22.045	1.00	46.24

2170	ND1	HIS	B	691	11.185	37.08	22.695	1.00	46.60
2171	CE1	HIS	B	691	12.319	37.31	23.33	1.00	46.83
2172	NE2	HIS	B	691	12.772	38.49	22.954	1.00	47.22
2173	C	HIS	B	691	8.198	36.79	19.584	1.00	41.36
2174	O	HIS	B	691	7.732	35.71	19.945	1.00	41.77
2175	N	ARG	B	692	7.497	37.69	18.904	1.00	40.51
2176	CA	ARG	B	692	6.108	37.46	18.531	1.00	40.58
2177	CB	ARG	B	692	5.585	38.62	17.68	1.00	41.97
2178	CG	ARG	B	692	4.103	38.54	17.334	1.00	44.31
2179	CD	ARG	B	692	3.748	39.58	16.287	1.00	46.39
2180	NE	ARG	B	692	4.433	39.31	15.024	1.00	48.87
2181	CZ	ARG	B	692	4.503	40.17	14.009	1.00	49.52
2182	NH1	ARG	B	692	3.928	41.36	14.099	1.00	50.67
2183	NH2	ARG	B	692	5.15	39.83	12.901	1.00	49.63
2184	C	ARG	B	692	5.99	36.15	17.748	1.00	39.77
2185	O	ARG	B	692	5.238	35.25	18.134	1.00	38.70
2186	N	LEU	B	693	6.739	36.05	16.652	1.00	38.99
2187	CA	LEU	B	693	6.718	34.85	15.816	1.00	39.44
2188	CB	LEU	B	693	7.804	34.92	14.735	1.00	38.36
2189	CG	LEU	B	693	7.65	35.94	13.602	1.00	38.71
2190	CD1	LEU	B	693	8.863	35.86	12.69	1.00	37.17
2191	CD2	LEU	B	693	6.38	35.65	12.815	1.00	37.74
2192	C	LEU	B	693	6.924	33.59	16.642	1.00	40.12
2193	O	LEU	B	693	6.275	32.57	16.412	1.00	40.20
2194	N	LEU	B	694	7.834	33.66	17.606	1.00	41.30
2195	CA	LEU	B	694	8.116	32.51	18.455	1.00	43.03
2196	CB	LEU	B	694	9.4	32.75	19.249	1.00	41.27
2197	CG	LEU	B	694	10.684	32.76	18.413	1.00	40.09
2198	CD1	LEU	B	694	11.845	33.25	19.251	1.00	39.04
2199	CD2	LEU	B	694	10.953	31.36	17.879	1.00	39.24
2200	C	LEU	B	694	6.967	32.19	19.407	1.00	45.64
2201	O	LEU	B	694	6.867	31.07	19.907	1.00	44.78
2202	N	GLN	B	695	6.098	33.17	19.645	1.00	49.29
2203	CA	GLN	B	695	4.964	32.98	20.55	1.00	53.51

2204	CB	GLN	B	695	4.348	34.33	20.927	1.00	53.94
2205	CG	GLN	B	695	5.333	35.37	21.451	1.00	54.96
2206	CD	GLN	B	695	6.079	34.93	22.698	1.00	55.61
2207	OE1	GLN	B	695	6.874	35.68	23.258	1.00	55.52
2208	NE2	GLN	B	695	5.828	33.7	23.138	1.00	55.62
2209	C	GLN	B	695	3.877	32.09	19.953	1.00	55.94
2210	O	GLN	B	695	3.046	31.55	20.681	1.00	55.76
2211	N	GLU	B	696	3.88	31.96	18.629	1.00	58.97
2212	CA	GLU	B	696	2.889	31.14	17.938	1.00	62.61
2213	CB	GLU	B	696	1.479	31.66	18.24	1.00	63.02
2214	CG	GLU	B	696	1.349	33.18	18.306	1.00	63.82
2215	CD	GLU	B	696	1.774	33.87	17.026	1.00	64.13
2216	OE1	GLU	B	696	1.142	33.63	15.977	1.00	64.51
2217	OE2	GLU	B	696	2.743	34.66	17.072	1.00	64.16
2218	C	GLU	B	696	3.104	31.1	16.429	1.00	64.98
2219	O	GLU	B	696	2.736	30.12	15.772	1.00	65.58
2220	N	GLY	B	697	3.699	32.15	15.883	1.00	67.35
2221	CA	GLY	B	697	3.946	32.2	14.454	1.00	70.03
2222	C	GLY	B	697	3.53	33.52	13.838	1.00	71.80
2223	O	GLY	B	697	3.13	34.45	14.543	1.00	71.76
2224	O	HOH	S	1	23.026	22.4	-2.192	1.00	19.60
2225	O	HOH	S	2	16.83	36.19	0.675	1.00	18.07
2226	O	HOH	S	3	22.154	35.44	11.146	1.00	15.63
2227	O	HOH	S	4	24.973	20.25	-2.261	1.00	20.14
2228	O	HOH	S	5	22.161	29.6	15.788	1.00	19.70
2229	O	HOH	S	6	24.965	31.5	-0.66	1.00	16.40
2230	O	HOH	S	7	10.844	33.69	-3.369	1.00	17.23
2231	O	HOH	S	8	22.447	38.7	-17.98	1.00	31.92
2232	O	HOH	S	9	17.526	31.03	1.265	1.00	14.10
2233	O	HOH	S	10	29.027	37.84	2.226	1.00	16.59
2234	O	HOH	S	11	16.149	33.62	0.874	1.00	17.71
2235	O	HOH	S	12	21.554	23.97	-0.428	1.00	13.97
2236	O	HOH	S	13	24.572	41.48	-5.871	1.00	19.10
2237	O	HOH	S	14	34.349	22.18	2.662	1.00	23.28

2238	O	HOH	S	15	23.974	19.69	-6.03	1.00	21.97
2239	O	HOH	S	16	12.346	31.08	-5.777	1.00	18.26
2240	O	HOH	S	17	17.302	24.21	0.483	1.00	21.48
2241	O	HOH	S	18	12.779	35.67	-4.261	1.00	15.87
2242	O	HOH	S	19	32.946	42.65	9.74	1.00	47.61
2243	O	HOH	S	20	6.647	45.31	0.256	1.00	32.40
2244	O	HOH	S	21	11.636	46.33	3.1	1.00	47.12
2245	O	HOH	S	22	15.387	32.46	-1.723	1.00	24.92
2246	O	HOH	S	23	15.179	49.11	-1.349	1.00	26.79
2247	O	HOH	S	24	17.323	27.72	27.462	1.00	23.87
2248	O	HOH	S	25	32.126	32.89	-0.975	1.00	24.24
2249	O	HOH	S	26	17.22	13.39	7.072	1.00	30.98
2250	O	HOH	S	27	17.61	52.48	-12.57	1.00	30.41
2251	O	HOH	S	28	11.598	28.45	0.826	1.00	27.74
2252	O	HOH	S	29	29.348	58.2	3.202	1.00	24.47
2253	O	HOH	S	30	20.33	34.13	24.733	1.00	27.25
2254	O	HOH	S	31	11.314	30.72	-3.163	1.00	29.15
2255	O	HOH	S	32	14.534	17.66	-8.919	1.00	23.07
2256	O	HOH	S	33	12.594	30.55	30.559	1.00	24.86
2257	O	HOH	S	34	4.997	18.18	3.778	1.00	28.69
2258	O	HOH	S	35	14.93	26.08	0.846	1.00	31.48
2259	O	HOH	S	36	26.37	38.41	-9.188	1.00	23.21
2260	O	HOH	S	37	1.85	51.46	-7.183	1.00	42.96
2261	O	HOH	S	38	30.499	11.23	5.931	1.00	32.46
2262	O	HOH	S	39	11.29	49.8	6.081	1.00	48.93
2263	O	HOH	S	40	20.535	16.89	-4.929	1.00	32.28
2264	O	HOH	S	41	24.859	35.08	-15.49	1.00	21.88
2265	O	HOH	S	42	7.686	40.68	3.298	1.00	37.33
2266	O	HOH	S	43	27.519	46.28	-18.33	1.00	37.96
2267	O	HOH	S	44	22.661	13.79	-4.577	1.00	49.60
2268	O	HOH	S	45	7.412	32.25	11.943	1.00	23.05
2269	O	HOH	S	46	31.273	40.98	1.303	1.00	31.68
2270	O	HOH	S	47	33.257	32.33	3.506	1.00	19.13
2271	O	HOH	S	48	6.534	16.95	5.915	1.00	23.85

2272	O	HOH	S	49	17.618	50.65	7.877	1.00	28.11
2273	O	HOH	S	50	20.823	9.387	10.717	1.00	28.29
2274	O	HOH	S	51	13.363	37.04	29.626	1.00	23.94
2275	O	HOH	S	52	9.174	18.86	-1.964	1.00	33.23
2276	O	HOH	S	53	23.557	48.69	-14.77	1.00	55.81
2277	O	HOH	S	54	33.983	34.75	2.856	1.00	26.86
2278	O	HOH	S	55	29.833	11	8.326	1.00	28.51
2279	O	HOH	S	57	11.766	42.24	23.635	1.00	42.57
2280	O	HOH	S	58	14.76	33.63	-4.189	1.00	32.75
2281	O	HOH	S	59	12.5	34.34	29.874	1.00	22.65
2282	O	HOH	S	60	28.126	41.87	-15.42	1.00	31.74
2283	O	HOH	S	61	26.365	40.53	-7.535	1.00	22.73
2284	O	HOH	S	62	22.279	46.65	-15.85	1.00	50.83
2285	O	HOH	S	63	7.178	15.42	0.05	1.00	44.46
2286	O	HOH	S	64	3.624	30.59	-0.214	1.00	36.39
2287	O	HOH	S	65	6.139	27.86	3.768	1.00	52.56
2288	O	HOH	S	66	31.097	55.49	8.217	1.00	30.35
2289	O	HOH	S	67	18.605	58.14	-1.051	1.00	47.14
2290	O	HOH	S	68	8.343	23.64	26.996	1.00	32.72
2291	O	HOH	S	69	19.685	57.59	-3.396	1.00	43.61
2292	O	HOH	S	70	20.943	28.28	33.357	1.00	40.59
2293	O	HOH	S	71	21.649	36.71	27.743	1.00	35.00
2294	O	HOH	S	72	31.539	42.79	3.263	1.00	30.88
2295	O	HOH	S	73	13.289	50.24	2.509	1.00	38.75
2296	O	HOH	S	74	19.123	53.23	5.431	1.00	37.22
2297	O	HOH	S	75	10.856	22.35	19.47	1.00	19.26
2298	O	HOH	S	76	4.014	20.49	2.2	1.00	37.71
2299	O	HOH	S	78	32.803	10.68	9.175	1.00	22.60
2300	O	HOH	S	79	15.982	27.46	-1.316	1.00	30.63
2301	O	HOH	S	80	6.778	41.32	9.974	1.00	45.09
2302	O	HOH	S	81	6.267	30.45	7.93	1.00	33.02
2303	O	HOH	S	82	19.319	14.91	21.654	1.00	42.45
2304	O	HOH	S	83	2.585	29.42	1.807	1.00	40.89
2305	O	HOH	S	84	2.194	49.14	-16.66	1.00	53.37

2306	O	HOH	S	85	36.352	8.69	3.311	1.00	40.82
2307	O	HOH	S	86	22.685	19.53	29.701	1.00	47.69
2308	O	HOH	S	87	33.974	34.64	0.26	1.00	31.56
2309	O	HOH	S	88	31.744	38.24	1.513	1.00	22.56
2310	O	HOH	S	89	5.825	37.89	6.408	1.00	48.05
2311	O	HOH	S	90	19.49	17.4	-8.965	1.00	38.26
2312	O	HOH	S	91	40.414	35.6	7.949	1.00	35.76
2313	O	HOH	S	92	15.402	46.87	15.762	1.00	39.90
2314	O	HOH	S	93	6.875	29.53	-13.41	1.00	40.19
2315	O	HOH	S	94	8.648	28.6	20.645	1.00	29.73
2316	O	HOH	S	95	22.063	37.44	22.081	1.00	37.50
2317	O	HOH	S	96	27.61	30.94	23.964	1.00	32.74
2318	O	HOH	S	97	10.971	31.16	27.918	1.00	24.96
2319	O	HOH	S	98	26.229	25.48	-11.89	1.00	41.41
2320	O	HOH	S	100	6.704	33.43	-14.58	1.00	36.10
2321	O	HOH	S	101	15.544	8.896	10.723	1.00	33.88
2322	O	HOH	S	102	16.493	16.84	-2.596	1.00	26.55
2323	O	HOH	S	103	28.351	28.27	12.338	1.00	43.77
2324	O	HOH	S	104	27.737	3.455	13.166	1.00	48.23
2325	O	HOH	S	105	24.873	39.51	-19.21	1.00	53.25
2326	O	HOH	S	106	12.972	44.58	-8.54	1.00	25.37
2327	O	HOH	S	107	20.643	61.57	2.015	1.00	57.43
2328	O	HOH	S	108	18.412	21.18	-12.7	1.00	30.69
2329	O	HOH	S	109	21.691	40.71	28.501	1.00	31.23
2330	O	HOH	S	111	37.452	24.33	8.574	1.00	43.15
2331	O	HOH	S	112	28.082	12.03	-2.83	1.00	35.13
2332	O	HOH	S	113	13.626	6.782	9.82	1.00	59.43
2333	O	HOH	S	114	29.219	47.39	-11.5	1.00	33.93
2334	O	HOH	S	115	37.194	25.42	11.265	1.00	49.29
2335	O	HOH	S	116	32.453	24.1	12.149	1.00	37.91
2336	O	HOH	S	117	20.069	18.41	-15.74	1.00	52.69
2337	O	HOH	S	118	37.303	36.57	3.605	1.00	50.95
2338	O	HOH	S	119	26.65	37.93	27.599	1.00	60.19
2339	O	HOH	S	120	40.042	37.14	6.054	1.00	62.83

2340	O	HOH	S	121	16.718	28.82	32.714	1.00	45.22
2341	O	HOH	S	122	15.637	14.39	-3	1.00	32.52
2342	O	HOH	S	123	25.337	43.41	12.302	1.00	46.21
2343	O	HOH	S	124	35.978	27.43	-0.068	1.00	39.51
2344	O	HOH	S	125	33.68	38.72	-6.927	1.00	55.40
2345	O	HOH	S	126	2.654	22.83	6.016	1.00	32.62
2346	O	HOH	S	127	21.42	16.3	32.91	1.00	56.84
2347	O	HOH	S	128	2.525	25.69	7.475	1.00	49.14
2348	O	HOH	S	129	38.283	26.64	7.527	1.00	36.28
2349	O	HOH	S	130	24.339	56.08	-3.205	1.00	42.51
2350	O	HOH	S	131	31.349	39.79	-15.87	1.00	43.44
2351	O	HOH	S	132	14.264	49.95	9.76	1.00	46.86
2352	O	HOH	S	133	29.477	46.34	-15.12	1.00	56.58
2353	O	HOH	S	134	13.24	46.59	14.288	1.00	30.39
2354	O	HOH	S	135	28.713	21.45	14.541	1.00	43.43
2355	O	HOH	S	136	29.863	19.83	16.145	1.00	53.77
2356	O	HOH	S	137	28.691	40.59	0.038	1.00	27.60
2357	O	HOH	S	138	31.992	29.57	17.933	1.00	52.12
2358	O	HOH	S	139	32.346	41.3	-7.206	1.00	48.91
2359	O	HOH	S	140	18.153	37.55	22.932	1.00	31.27
2360	O	HOH	S	141	16.88	57.73	-7.178	1.00	36.07
2361	O	HOH	S	142	3.616	38.62	3.9	1.00	63.76
2362	O	HOH	S	143	18.536	13.34	-5.108	1.00	59.11
2363	O	HOH	S	144	6.14	50.93	-15.59	1.00	38.96
2364	O	HOH	S	145	14.732	25.97	29.458	1.00	32.23
2365	O	HOH	S	146	21.729	19.32	-8.314	1.00	36.70
2366	O	HOH	S	147	8.169	16.53	17.709	1.00	58.27
2367	O	HOH	S	148	11.709	32.98	0.499	1.00	36.22
2368	O	HOH	S	149	13.578	48.33	0.597	1.00	37.61
2369	O	HOH	S	150	12.376	12.47	17.052	1.00	62.89
2370	O	HOH	S	151	9.626	31.89	1.206	1.00	68.72
2371	O	HOH	S	152	28.153	19.15	18.731	1.00	42.30
2372	O	HOH	S	153	32.498	45.94	-7.499	1.00	37.61
2373	O	HOH	S	154	24.755	0.891	18.958	1.00	66.75

2374	O	HOH	S	155	39.681	22.65	2.229	1.00	35.42
2375	O	HOH	S	156	13.536	52.85	2.389	1.00	37.57
2376	O	HOH	S	157	8.317	48.95	2.546	1.00	73.06
2377	O	HOH	S	158	8.644	28.04	-12.59	1.00	33.91
2378	O	HOH	S	159	2.877	30.15	4.135	1.00	62.49
2379	O	HOH	S	160	31.522	7.355	4.7	1.00	35.95
2380	O	HOH	S	161	5.863	26.35	22.68	1.00	39.01
2381	O	HOH	S	162	7.589	46.35	-19.67	1.00	50.76
2382	O	HOH	S	163	22.983	9.848	-2.49	1.00	64.92
2383	O	HOH	S	164	6.674	37.22	8.925	1.00	35.74
2384	O	HOH	S	165	1.66	40.66	10.72	1.00	68.96
2385	O	HOH	S	166	37.85	28.01	11.075	1.00	29.28
2386	O	HOH	S	167	2.367	30.07	11.169	1.00	47.90
2387	O	HOH	S	168	22.807	6.884	24.267	1.00	50.27
2388	O	HOH	S	169	25.253	24.05	-9.518	1.00	56.25
2389	O	HOH	S	170	31.929	40.72	-4.78	1.00	43.99
2390	O	HOH	S	171	29.051	32.12	-14.16	1.00	48.37
2391	O	HOH	S	172	6.854	24.41	13.632	1.00	30.86
2392	O	HOH	S	173	31.121	26.37	-0.287	1.00	26.16
2393	O	HOH	S	174	26.425	4.757	16.289	1.00	46.62
2394	O	HOH	S	175	30.245	52.79	-1.002	1.00	62.86
2395	O	HOH	S	176	11.266	25.3	-15.97	1.00	30.67
2396	O	HOH	S	177	8.232	22.79	-8.256	1.00	36.47
2397	O	HOH	S	178	32.73	30.85	1.133	1.00	29.48
2398	O	HOH	S	179	12.168	13.53	-6.965	1.00	54.81
2399	O	HOH	S	181	9.981	18.58	-15.66	1.00	52.49
2400	O	HOH	S	182	2.592	15.84	3.846	1.00	36.47
2401	O	HOH	S	184	16.07	21.67	25.099	1.00	36.38
2402	O	HOH	S	185	9.58	53.07	5.376	1.00	51.65
2403	O	HOH	S	186	9.863	33.55	29.136	1.00	41.08
2404	O	HOH	S	187	28.882	9.516	-2.636	1.00	43.51
2405	O	HOH	S	188	28.982	14.1	-1.733	1.00	52.94
2406	O	HOH	S	189	8.611	16.55	11.998	1.00	34.51
2407	O	HOH	S	190	12.85	16.63	-1.121	1.00	38.29

2408	O	HOH	S	191	28.378	56.86	-0.306	1.00	70.56
2409	O	HOH	S	192	21.342	14.62	28.328	1.00	75.81
2410	O	HOH	S	193	29.531	7.961	13.212	1.00	47.28
2411	O	HOH	S	194	32.953	32.46	15.308	1.00	53.06
2412	O	HOH	S	195	6.057	23.07	15.892	1.00	44.59
2413	O	HOH	S	196	32.031	9.855	17.068	1.00	61.54
2414	O	HOH	S	197	31.244	15.54	16.59	1.00	47.53
2415	O	HOH	S	198	25.439	9.787	20.81	1.00	55.35
2416	O	HOH	S	199	17.929	17.39	-4.951	1.00	38.99
2417	O	HOH	S	200	20.119	56.57	-12.07	1.00	34.77
2418	O	HOH	S	201	5.206	29.9	4.996	1.00	54.91
2419	O	HOH	S	202	14.253	59.12	-6.767	1.00	57.78
2420	O	HOH	S	203	2.327	36.03	19.271	1.00	71.38
2421	O	HOH	S	205	25.908	29.01	30.674	1.00	45.68
2422	O	HOH	S	206	6.998	27.65	7.373	1.00	33.37
2423	O	HOH	S	207	29.909	10.26	3.633	1.00	28.69
2424	O	HOH	S	208	3.221	39.57	9.013	1.00	64.29
2425	O	HOH	S	209	11.662	26.03	31.453	1.00	30.92
2426	O	HOH	S	210	30.602	43.9	-10.34	1.00	35.47
2427	O	HOH	S	211	5.674	19.99	12.478	1.00	36.93
2428	O	HOH	S	212	8.997	8.066	12.548	1.00	44.27
2429	O	HOH	S	213	18.565	1.299	23.321	1.00	53.87
2430	O	HOH	S	214	14.123	50.52	-14.45	1.00	54.64
2431	O	HOH	S	215	18.959	15.48	28.395	1.00	71.59
2432	O	HOH	S	216	0.665	37.38	17.683	1.00	49.95
2433	O	HOH	S	217	26.863	55.57	-2.207	1.00	46.16
2434	O	HOH	S	218	6.158	22.9	11.742	1.00	31.87
2435	O	HOH	S	219	9.888	16.38	-1.719	1.00	36.68
2436	O	HOH	S	220	30.266	27.84	23.674	1.00	53.45
2437	O	HOH	S	221	30.769	47.55	-1.614	1.00	42.34
2438	O	HOH	S	222	32.195	35.01	15.035	1.00	44.29
2439	O	HOH	S	223	10.286	34.65	-0.758	1.00	25.15
2440	O	HOH	S	224	4.88	17.84	16.029	1.00	58.71
2441	O	HOH	S	225	5.737	41.57	7.23	1.00	41.48

2442	O	HOH	S	226	24.968	27.07	-7.625	1.00	61.37
2443	O	HOH	S	227	26.43	10.73	26.093	1.00	47.70
2444	O	HOH	S	228	9.402	26.41	28.179	1.00	51.51
2445	O	HOH	S	229	22.501	23.96	-9.399	1.00	43.79
2446	O	HOH	S	232	36.306	31.18	7.127	1.00	49.35
2447	O	HOH	S	233	16.063	56.54	4.731	1.00	47.51
2448	O	HOH	S	234	9.113	46	15.205	1.00	51.54
2449	O	HOH	S	236	22.85	16.02	-6.845	1.00	48.61
2450	O	HOH	S	237	4.561	37.73	10.108	1.00	63.61
2451	O	HOH	S	238	8.317	20.22	-8.658	1.00	40.62
2452	O	HOH	S	239	26.545	17.09	26.547	1.00	60.48
2453	O	HOH	S	240	18.438	52.12	-15.97	1.00	68.74
2454	O	HOH	S	241	15.737	11.25	6.148	1.00	40.27
2455	O	HOH	S	242	-2.46	33.66	15.319	1.00	56.63
2456	O	HOH	S	243	9.254	37.4	27.214	1.00	50.70
2457	O	HOH	S	244	22.874	5.448	-0.368	1.00	56.93
2458	O	HOH	S	245	1.408	28.07	19.082	1.00	54.97
2459	O	HOH	S	246	29.407	5.692	12.371	1.00	46.23
2460	O	HOH	S	247	21.392	2.016	21.068	1.00	54.78
2461	O	HOH	S	248	3.142	52.17	-19.3	1.00	61.95
2462	O	HOH	S	249	22.021	57.55	-0.613	1.00	48.17
2463	O	HOH	S	250	13.662	3.611	13.009	1.00	43.82
2464	O	HOH	S	251	19.193	16.6	19.469	1.00	31.39
2465	O	HOH	S	252	3.331	33.52	6.6	1.00	47.67
2466	O	HOH	S	253	10.792	2.983	19.468	1.00	70.14
2467	O	HOH	S	254	16.787	17.52	20.507	1.00	63.73
2468	O	HOH	S	255	2.619	44.64	16.706	1.00	56.53
2469	O	HOH	S	256	27.869	14.32	18.171	1.00	41.98
2470	O	HOH	S	257	31.415	45.49	-13.52	1.00	53.59
2471	O	HOH	S	258	31.255	35.57	-11.97	1.00	33.65
2472	O	HOH	S	259	21.689	4.451	26.354	1.00	52.63
2473	O	HOH	S	260	10.441	20.46	21.585	1.00	35.08
2474	O	HOH	S	261	17.807	18.05	18.034	1.00	49.80
2475	O	HOH	S	262	12.939	41.2	25.86	1.00	49.78

2476	O	HOH	S	263	11.831	38.27	27.695	1.00	41.47
2477	O	HOH	S	264	21.694	14.49	25.644	1.00	49.41
2478	O	HOH	S	265	3.278	19.42	-21.24	1.00	58.93
2479	O	HOH	S	266	32.139	44.55	-1.767	1.00	63.10
2480	O	HOH	S	267	30.536	19.71	26.309	1.00	56.72
2481	O	HOH	S	268	1.033	38.18	8.349	1.00	69.65
2482	O	HOH	S	269	15.677	56.47	-11.13	1.00	45.85
2483	O	HOH	S	270	9.631	49.19	-12.73	1.00	31.76
2484	O	HOH	S	271	26.281	33.95	12.002	1.00	28.74
2485	O	HOH	S	272	16.307	55.36	-6.008	1.00	48.50
2486	O	HOH	S	273	35.226	25.13	1.967	1.00	37.37
2487	O	HOH	S	274	34.15	31.09	10.684	1.00	35.88
2488	O	HOH	S	275	9.81	12.1	-10.1	1.00	42.96
2489	O	HOH	S	277	31.321	17.79	15.555	1.00	54.02
2490	O	HOH	S	278	6.023	17.62	1.258	1.00	32.48
2491	O	HOH	S	279	10.646	28.67	26.826	1.00	33.27
2492	O	HOH	S	280	33.133	28.2	0.795	1.00	32.26
2493	O	HOH	S	281	4.679	49.52	-17.39	1.00	56.01
2494	O	HOH	S	282	19.923	38.29	25.079	1.00	52.01
2495	O	HOH	S	283	17.06	16.72	-7.694	1.00	44.99
2496	O	HOH	S	284	8.155	32.99	31.053	1.00	38.13
2497	O	HOH	S	285	15.353	23.01	31.936	1.00	47.35
2498	O	HOH	S	286	37.587	33.19	10.823	1.00	50.51
2499	O	HOH	S	287	26.366	26.07	14.494	1.00	43.81
2500	O	HOH	S	288	9.308	11.77	3.313	1.00	52.95
2501	O	HOH	S	289	29.889	5.039	4.211	1.00	39.94
2502	O	HOH	S	290	21.608	63.69	5.695	1.00	47.51
2503	O	HOH	S	291	5.878	51.06	-5.441	1.00	57.81
2504	O	HOH	S	292	4.217	31.18	9.122	1.00	34.04
2505	O	HOH	S	293	20.204	52.12	-12.15	1.00	32.14
2506	O	HOH	S	294	31.777	46.88	-9.872	1.00	37.63
2507	O	HOH	S	295	29.367	16.37	18.828	1.00	47.88
2508	O	HOH	S	296	7.053	22.51	23.361	1.00	49.62
2509	O	HOH	S	297	10.448	17.83	24.905	1.00	45.38

2510	O	HOH	S	298	22.727	21.64	-7.856	1.00	44.54
2511	O	HOH	S	299	41.752	38.42	4.331	1.00	51.42
2512	O	HOH	S	300	28.35	29.18	29.86	1.00	35.37
2513	O	HOH	S	301	19.875	8.686	8.347	1.00	36.88
2514	O	HOH	S	302	30.241	47.82	14.46	1.00	52.48
2515	O	HOH	S	303	38.107	31.69	-0.089	1.00	48.80
2516	O	HOH	S	304	29.435	19.53	22.017	1.00	48.53
2517	O	HOH	S	305	28.231	17.78	23.534	1.00	49.19
2518	O	HOH	S	306	25.102	25.86	30.666	1.00	50.04
2519	O	HOH	S	307	20.946	24.31	-13.66	1.00	35.02
2520	O	HOH	S	308	27.296	9.199	14.576	1.00	37.16
2521	O	HOH	S	309	5.593	44.21	15.509	1.00	46.00
2522	O	HOH	S	310	1.445	15.84	16.482	1.00	48.72
2523	O	HOH	S	311	31.898	52.12	-9.291	1.00	36.65
2524	O	HOH	S	312	2.78	26.87	21.407	1.00	37.83
2525	O	HOH	S	313	10.829	21.85	1.47	1.00	38.42
2526	O	HOH	S	314	25.186	43.65	22.198	1.00	39.85
2527	O	HOH	S	315	10.029	44.29	3.158	1.00	61.53
2528	O	HOH	S	316	25.08	12.34	-5.224	1.00	49.90
2529	O	HOH	S	317	24.701	26.06	34.199	1.00	51.37
2530	O	HOH	S	318	17.657	17.78	-11.97	1.00	54.01
2531	O	HOH	S	319	21.669	9.232	-4.594	1.00	50.75
2532	O	HOH	S	320	12.831	30.46	-0.73	1.00	46.31
2533	O	HOH	S	321	-0.839	31.74	16.05	1.00	49.15
2534	O	HOH	S	322	11.333	25.16	29.142	1.00	54.91
2535	O	HOH	S	323	38.448	33.36	4.415	1.00	47.87
2536	O	HOH	S	324	29.755	48.47	-20.47	1.00	61.21
2537	O	HOH	S	325	19.876	22.91	34.487	1.00	53.69
2538	O	HOH	S	326	6.159	6.348	12.404	1.00	45.47
2539	O	HOH	S	327	24.803	24.04	-13.67	1.00	41.36
2540	O	HOH	S	328	34.41	33.84	13.722	1.00	48.67
2541	O	HOH	S	330	28.488	24.85	15.172	1.00	42.44
2542	O	HOH	S	331	18.756	10.01	-0.302	1.00	47.49
2543	O	HOH	S	332	27.919	33.32	15.964	1.00	46.60

2544	O	HOH	S	333	28.084	54.17	-9.919	1.00	47.31
2545	O	HOH	S	334	6.66	20.06	17.321	1.00	66.41
2546	O	HOH	S	335	9.177	51.42	-1.091	1.00	50.92
2547	O	HOH	S	336	26.133	49.98	-13.04	1.00	44.73
2548	O	HOH	S	337	6.461	-15	10.655	1.00	50.61
2549	O	HOH	S	338	27.448	21.32	29.977	1.00	46.70
2550	O	HOH	S	339	-2.375	39.03	9.478	1.00	48.95
2551	O	HOH	S	340	39.666	-34.71	11.042	1.00	54.77
2552	O	HOH	S	341	31.504	4.157	11.722	1.00	38.27
2553	O	HOH	S	342	30.223	43.44	12.537	1.00	56.22
2554	O	HOH	S	343	31.793	6.842	14.029	1.00	49.62
2555	O	HOH	S	344	34.165	36.36	-11.48	1.00	54.81
2556	O	HOH	S	345	16.345	29.91	-0.844	1.00	50.86
2557	O	HOH	S	346	16.038	14.04	-0.096	1.00	26.81
2558	O	HOH	S	347	35.56	39.29	6.896	1.00	58.70
2559	O	HOH	S	348	7.207	18.78	-13.36	1.00	48.09
2560	O	HOH	S	349	4.347	25.73	17.608	1.00	48.32
2561	O	HOH	S	350	23.981	49.9	20.29	1.00	45.46
2562	O	HOH	S	351	-1.311	39.18	20.561	1.00	47.06
2563	O	HOH	S	352	29.438	35.08	-13.57	1.00	51.53
2564	O	HOH	S	353	22.157	11.96	-8.267	1.00	58.38
2565	O	HOH	S	354	28.535	23.39	-8.407	1.00	38.50
2566	O	HOH	S	355	16.02	7.615	25.043	1.00	63.84
2567	O	HOH	S	356	2.323	34.05	2.822	1.00	52.94
2568	O	HOH	S	357	14.88	19.56	25.915	1.00	44.98
2569	O	HOH	S	358	33.923	47.33	-12.62	1.00	52.85
2570	O	HOH	S	359	27.496	24.78	30.413	1.00	48.33
2571	O	HOH	S	360	20.476	43.25	26.095	1.00	52.94
2572	O	HOH	S	361	28.282	37.79	30.539	1.00	62.99
2573	O	HOH	S	362	27.472	34.09	-15.38	1.00	50.71
2574	O	HOH	S	363	25.666	34.54	30.416	1.00	54.08
2575	O	HOH	S	364	29.779	1.14	1.301	1.00	59.34
2576	O	HOH	S	365	5.434	39.02	22.161	1.00	47.10
2577	O	HOH	S	366	5.05	16.76	20.069	1.00	60.26

2578	O	HOH	S	367	18.636	55.72	-4.804	1.00	55.62
2579	O	HOH	S	368	32.684	59.06	10.827	1.00	39.90
2580	O	HOH	S	369	28.244	51.07	-11.91	1.00	52.57
2581	O	HOH	S	370	11.589	51.23	-1.777	1.00	63.06
2582	O	HOH	S	371	2.98	19.43	-24.51	1.00	45.57
2583	O	HOH	S	372	22.088	60	-1.466	1.00	61.45
2584	O	HOH	S	373	22.665	43.26	31.048	1.00	47.28
2585	O	HOH	S	374	30.445	38.97	29.886	1.00	57.25
2586	O	HOH	S	375	35.859	38.01	1.977	1.00	61.81
2587	O	HOH	S	376	6.112	31.91	-17.26	1.00	49.61
2588	O	HOH	S	377	6.721	15.6	-22.4	1.00	59.42
2589	O	HOH	S	378	12.118	1.192	18.305	1.00	48.35
2590	O	HOH	S	379	4.24	32.09	1.805	1.00	44.18
2591	O	HOH	S	380	29.696	35.08	27.75	1.00	55.76
2592	O	HOH	S	381	26.359	7.481	25.027	1.00	51.90
2593	O	HOH	S	382	9.133	46.89	3.888	1.00	56.70
2594	O	HOH	S	383	10.643	46.44	-20.34	1.00	37.21
2595	O	HOH	S	384	8.232	48.96	17.207	1.00	59.01
2596	O	HOH	S	385	20.326	15.01	-8.821	1.00	55.36
2597	O	HOH	S	386	19.253	-0.131	16.57	1.00	45.30
2598	O	HOH	S	387	7.34	49.8	-0.68	1.00	55.02
2599	O	HOH	S	388	2.512	47.88	0.707	1.00	48.12
2600	O	HOH	S	389	13.153	54.6	-2.131	1.00	53.44
2601	O	HOH	S	390	17.487	16.51	30.198	1.00	49.11
2602	O	HOH	S	391	20.116	10.78	23.265	1.00	55.34
2603	O	HOH	S	392	23.496	12.69	26.104	1.00	62.62
2604	O	HOH	S	393	20.396	47.11	12.135	1.00	51.92
2605	O	HOH	S	394	9.042	10.92	17.744	1.00	57.21
2606	O	HOH	S	395	15.086	15.2	30.474	1.00	56.74
2607	O	HOH	S	396	27.824	7.29	-8.552	1.00	49.75
2608	O	HOH	S	397	-1.167	31.36	18.711	1.00	53.14
2609	O	HOH	S	398	7.302	35.54	28.016	1.00	61.44
2610	O	HOH	S	399	14.214	16.7	-13.22	1.00	42.98
2611	O	HOH	S	400	20.092	59.9	-2.921	1.00	54.66

2612	O	HOH	S	401	28.927	1.994	14.98	1.00	47.04
2613	O	HOH	S	402	14.185	28.7	31.582	1.00	59.65
2614	O	HOH	S	403	20.834	52.48	14.019	1.00	61.68
2615	O	HOH	S	404	13.279	5.355	25.439	1.00	52.09
2616	O	HOH	S	405	26.886	59.65	-2.846	1.00	46.54
2617	O	HOH	S	406	11.357	5.386	16.734	1.00	45.29
2618	O	HOH	S	407	30.634	57.68	11.14	1.00	63.95
2619	O	HOH	S	408	33.859	39.18	-13.25	1.00	54.28
2620	O	HOH	S	409	16.114	14.41	-7.014	1.00	46.14
2621	O	HOH	S	410	37.72	38.28	6.176	1.00	64.28
2622	O	HOH	S	411	6.555	42.04	-19.44	1.00	48.56
2623	C1A	735	C	1	19.341	40.73	3.993	1.00	15.91
2624	O1C	735	C	1	18.239	40.2	4.31	1.00	17.26
2625	O1B	735	C	1	20.381	40.5	4.658	1.00	17.17
2626	C1D	735	C	1	19.457	41.69	2.755	1.00	14.73
2627	C1X	735	C	1	19.835	43.1	3.255	1.00	16.66
2628	C1Y	735	C	1	18.085	41.87	1.978	1.00	16.99
2629	O1E	735	C	1	20.62	41.22	1.905	1.00	15.62
2630	C1F	735	C	1	20.412	40.1	1.046	1.00	12.70
2631	C1G	735	C	1	20.444	40.32	-0.337	1.00	16.64
2632	C1I	735	C	1	20.235	39.25	-1.206	1.00	15.86
2633	C1K	735	C	1	19.982	37.9	-0.694	1.00	15.12
2634	C1J	735	C	1	19.956	37.68	0.701	1.00	15.25
2635	C1H	735	C	1	20.17	38.77	1.574	1.00	16.34
2636	C1L	735	C	1	19.737	36.71	-1.661	1.00	16.46
2637	N1M	735	C	1	19.038	37.26	-2.855	1.00	16.48
2638	C2A	735	C	1	17.688	37.38	-3.024	1.00	19.45
2639	O2A	735	C	1	16.891	37	-2.138	1.00	20.40
2640	S2C	735	C	1	15.434	38.08	-4.377	1.00	18.50
2641	C2B	735	C	1	17.146	37.95	-4.199	1.00	18.76
2642	C2D	735	C	1	17.789	38.48	-5.386	1.00	19.70
2643	C2G	735	C	1	19.304	38.59	-5.689	1.00	20.26
2644	N2E	735	C	1	16.929	38.94	-6.305	1.00	17.68
2645	C2F	735	C	1	15.613	38.79	-5.935	1.00	19.94

2646	C2H	735	C	1	14.527	39.19	-6.734	1.00	21.71
2647	C2J	735	C	1	13.172	39	-6.28	1.00	20.47
2648	C2L	735	C	1	12.08	39.39	-7.09	1.00	22.73
2649	C2M	735	C	1	12.3	39.99	-8.38	1.00	20.47
2650	C2K	735	C	1	13.648	40.19	-8.827	1.00	23.90
2651	C2I	735	C	1	14.733	39.8	-8.026	1.00	22.13
2652	C2N	735	C	1	11.109	40.43	-9.297	1.00	25.97
2653	F2P	735	C	1	10.97	39.5	-10.3	1.00	31.88
2654	F2Q	735	C	1	9.921	40.5	-8.624	1.00	31.88
2655	F2O	735	C	1	11.341	41.65	-9.859	1.00	31.88

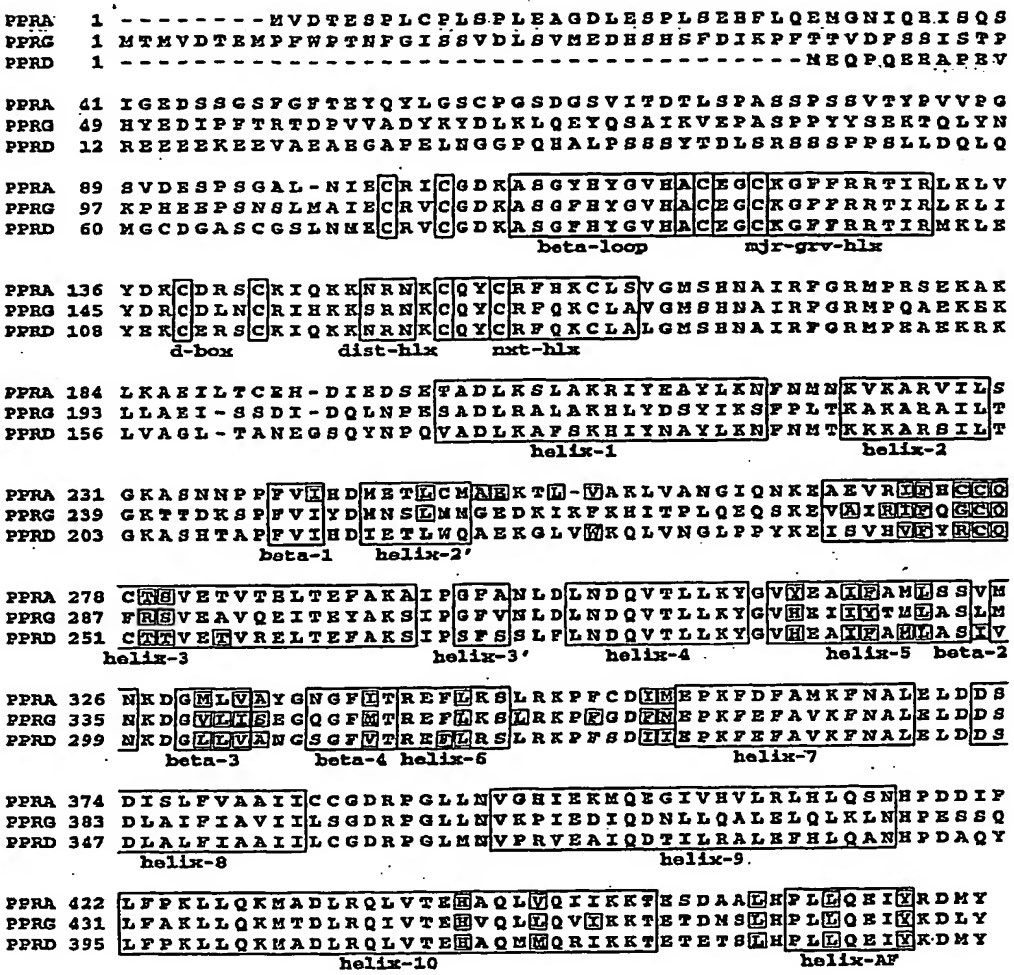


TABLE 4

It will be understood that various details of the invention may be changed without departing from the scope of the invention. Furthermore, the foregoing description is for the purpose of illustration only, and not for the purpose of limitation—the invention being defined by the claims.

CLAIMS

What is claimed is:

1. A substantially pure PPARα ligand binding domain polypeptide in crystalline form.

2. The polypeptide of claim 1, wherein the crystalline form has lattice constants of a = 61.3 Å, b = 103.5 Å, c = 49.9 Å, α = 90°, β = 90°, γ = 90°.

3. The polypeptide of claim 1 or 2, wherein the crystalline form is an orthorhombic crystalline form.

4. The polypeptide of claim 1 or 2, wherein the crystalline form has a space group of $P2_12_12$.

5. The polypeptide of claim 1 or 2, wherein the PPARα ligand binding domain polypeptide has the amino acid sequence shown in SEQ ID NO: 4.

6. The polypeptide of claim 1 or 2, wherein the PPARα ligand binding domain polypeptide is in complex with a ligand.

7. The polypeptide of claim 1 or 2, wherein the PPARα ligand binding domain has a crystalline structure further characterized by the coordinates corresponding to Table 2.

8. The polypeptide of claim 1 or 2, wherein the crystalline form contains one PPARα ligand binding domain polypeptide in the asymmetric unit.

9. The polypeptide of claim 1 or 2, wherein the crystalline form is such that the three-dimensional structure of the crystallized PPARα ligand

binding domain polypeptide can be determined to a resolution of about 1.8 Å or better.

10. The polypeptide of claim 1 or 2, wherein the crystalline form contains one or more atoms having a molecular weight of 40 grams/mol or greater.

11. The polypeptide of claim 1, wherein the crystalline form has lattice constants of a = 95.58 Å, b = 122.06 Å, c = 122.10 Å, α = 90°, β = 90°, γ = 90°.

12. The polypeptide of claim 1 or 11, wherein the crystalline form is an orthorhombic crystalline form.

13. The polypeptide of claim 1 or 11, wherein the crystalline form has a space group of $P2_12_12_1$.

14. The polypeptide of claim 1 or 11, wherein the PPARα ligand binding domain polypeptide has the amino acid sequence shown in SEQ ID NO: 4.

15. The polypeptide of claim 1 or 11, wherein the crystalline form contains four PPARα ligand binding domain polypeptides in the asymmetric unit.

16. The polypeptide of claim 1 or 11, wherein the crystalline form is such that the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide can be determined to a resolution of about 2.5 Å or better.

17. The polypeptide of claim 1 or 11, wherein the crystalline form contains one or more atoms having a molecular weight of 40 grams/mol or greater.

18. A method for determining the three-dimensional structure of a crystallized PPARα ligand binding domain polypeptide to a resolution of about 1.8 Å or better, the method comprising:

(a) crystallizing a PPARα ligand binding domain polypeptide; and

(b) analyzing the PPARα ligand binding domain polypeptide to determine the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide, whereby the three-dimensional structure of a crystallized PPARα ligand binding domain polypeptide is determined to a resolution of about 1.8 Å or better.

19. The method of claim 18, wherein the analyzing is by X-ray diffraction.

20. The method of claim 18, wherein the crystallization is accomplished by the hanging drop vapor diffusion method, and wherein the PPARα ligand binding domain is mixed with an equal volume of reservoir.

21. The method of claim 20, wherein the reservoir comprises 4-8% PEG 3350, 100-200mM NaF, and 12-16% 2,5 hexanediol.

22. The method of claim 20, wherein the reservoir comprises 50 mM bis-tris-propane, 4-6% PEG 3350, 150 mM $NaNO_3$, 16% 2,5 hexanediol and 1-3 mM YCl.

23. A method of generating a crystallized PPARα ligand binding domain polypeptide, the method comprising:

(a) incubating a solution comprising a PPARα ligand binding domain with an equal volume of reservoir; and

(b) crystallizing the PPARα ligand binding domain polypeptide using the hanging drop method, whereby a crystallized PPARα ligand binding domain polypeptide is generated.

24. A crystallized PPARα ligand binding domain polypeptide produced by the method of claim 23.

25. A method of designing a modulator of a PPAR polypeptide, the method comprising:

(a) designing a potential modulator of a PPAR polypeptide that will make interactions with amino acids in the ligand binding site based upon a crystalline structure of a PPARα ligand binding domain polypeptide;

(b) synthesizing the modulator; and

(c) determining whether the potential modulator modulates the activity of the PPAR polypeptide, whereby a modulator of a PPAR polypeptide is designed.

26. A method of designing a modulator that selectively modulates the activity of a PPAR polypeptide the method comprising:

(a) obtaining a crystalline form of a PPARα ligand binding domain polypeptide;

(b) evaluating the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide; and

(c) synthesizing a potential modulator based on the three-dimensional crystal structure of the crystallized PPARα ligand binding domain polypeptide, whereby a modulator that selectively modulates the activity of a PPARα polypeptide is designed.

27. The method of claim 26, wherein the method further comprises contacting a PPARα ligand binding domain polypeptide with the potential modulator, and assaying the PPARα ligand binding domain polypeptide for binding of the potential modulator, for a change in activity of the PPARα ligand binding domain polypeptide, or both.

28. The method of claim 26, wherein the crystalline form is in orthorhombic form.

29. The method of claim 28, wherein the crystalline form is such that the three-dimensional structure of the crystallized PPARα ligand binding domain polypeptide can be determined to a resolution of about 1.8 Å or better.

30. A method of screening a plurality of compounds for a modulator of a PPAR ligand binding domain polypeptide, the method comprising:

(a) providing a library of test samples;

(b) contacting a crystalline PPARα ligand binding domain polypeptide with each test sample;

(c) detecting an interaction between a test sample and the crystalline PPARα ligand binding domain polypeptide;

(d) identifying a test sample that interacts with the crystalline PPARα ligand binding domain polypeptide; and

(e) isolating a test sample that interacts with the crystalline PPARα ligand binding domain polypeptide, whereby a plurality of compounds is screened for a modulator of a PPAR ligand binding domain polypeptide.

31. The method of claim 30, wherein the test samples are bound to a substrate.

32. The method of claim 30, wherein the test samples are synthesized directly on a substrate.

33. A method for identifying a PPAR modulator, the method comprising:

(a) providing atomic coordinates of a PPARα ligand binding domain to a computerized modeling system;and

(b) modeling ligands that fit spatially into the binding pocket of the PPARα ligand binding domain to thereby identify a PPAR modulator, whereby a PPAR modulator is identified.

34. The method of claim 33, wherein the method further comprises identifying in an assay for PPAR-mediated activity a modeled ligand which increases or decreases the activity of the PPAR.

35. A method of identifying a PPARα modulator that selectively modulates the activity of a PPARα polypeptide compared to other polypeptides, the method comprising:

(a) providing atomic coordinates of a PPARα ligand binding domain to a computerized modeling system; and

(b) modeling a ligand that fits into the binding pocket of a PPARα ligand binding domain and that interacts with conformationally constrained residues of a PPARα conserved among PPAR subtypes, whereby a PPARα modulator that selectively modulates the activity of a PPARα polypeptide compared to other polypeptides.

36. The method of claim 35, wherein the method further comprises identifying in a biological assay for PPARα activity a modeled ligand that selectively binds to said PPARα and increases or decreases the activity of said PPARα.

37. A method of designing a modulator of a PPAR polypeptide, the method comprising:

(a) selecting a candidate PPAR ligand;

(b) determining which amino acid or amino acids of a PPAR polypeptide interact with the ligand using a three-dimensional model of a crystallized protein comprising a PPARα LBD;

(c) identifying in a biological assay for PPAR activity a degree to which the ligand modulates the activity of the PPAR polypeptide;

(d) selecting a chemical modification of the ligand wherein the interaction between the amino acids of the PPAR polypeptide and the ligand is predicted to be modulated by the chemical modification;

(e) performing the chemical modification on the ligand to form a modified ligand;

(f) contacting the modified ligand with the PPAR polypeptide;

(g) identifying in a biological assay for PPAR activity a degree to which the modified ligand modulates the biological activity of the PPAR polypeptide; and

(h) comparing the biological activity of the PPAR polypeptide in the presence of modified ligand with the biological activity of the PPAR polypeptide in the presence of the unmodified ligand, whereby a modulator of a PPAR polypeptide is designed.

38. The method of claim 37, wherein the PPAR polypeptide is a PPARα polypeptide.

39. The method of claim 37, wherein the three-dimensional model of a crystallized protein is a PPARα LBD polypeptide with a bound ligand.

40. The method of claim 37, wherein the method further comprises repeating steps (a) through (f), if the biological activity of the PPAR polypeptide in the presence of the modified ligand varies from the biological activity of the PPAR polypeptide in the presence of the unmodified ligand.

41. An assay method for identifying a compound that inhibits binding of a ligand to a PPAR polypeptide, the assay method comprising:

(a) incubating a PPAR polypeptide with a ligand in the presence of a test inhibitor compound;

(b) determining an amount of ligand that is bound to the PPAR polypeptide, wherein decreased binding of ligand to the PPAR protein in the presence of the test inhibitor compound relative to binding of ligand in the absence of the test inhibitor compound is indicative of inhibition; and

(c) identifying the test compound as an inhibitor of ligand binding if decreased ligand binding is observed, whereby a compound that inhibits binding of a ligand to a PPAR polypeptide is identified.

42. A method of identifying a PPAR modulator that selectively modulates the biological activity of one PPAR subtype compared to PPARα, the method comprising:

(a) providing an atomic structure coordinate set describing a PPARα ligand binding domain structure and at least one other atomic structure coordinate set describing a PPAR ligand binding domain, each ligand binding domain comprising a ligand binding site;

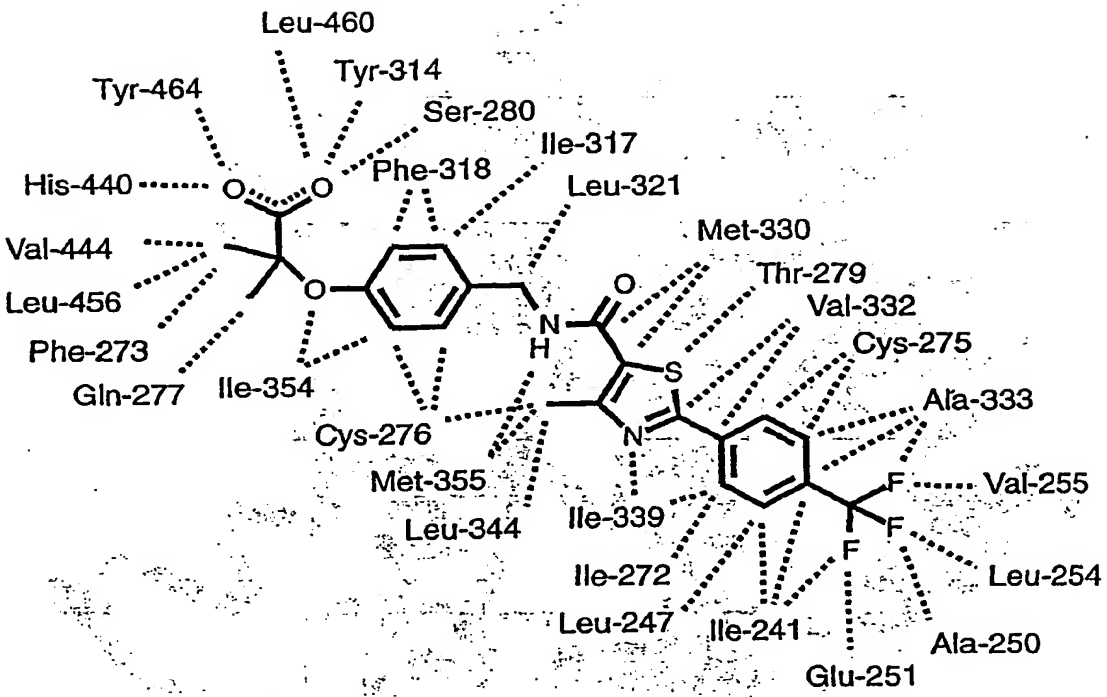
(b) comparing the PPAR atomic structure coordinate sets to identify at least one diference between the sets;

(c) designing a candidate ligand predicted to interact with the difference of step (b);

(d) synthesizing the candidate ligand; and

(e) testing the synthesized candidate ligand for an ability to selectively modulate a PPAR subtype as compared to PPARα, whereby a PPAR modulator that selectively modulates the biological activity of one PPAR subtype compared to PPARα is identified.

FIGURE 1



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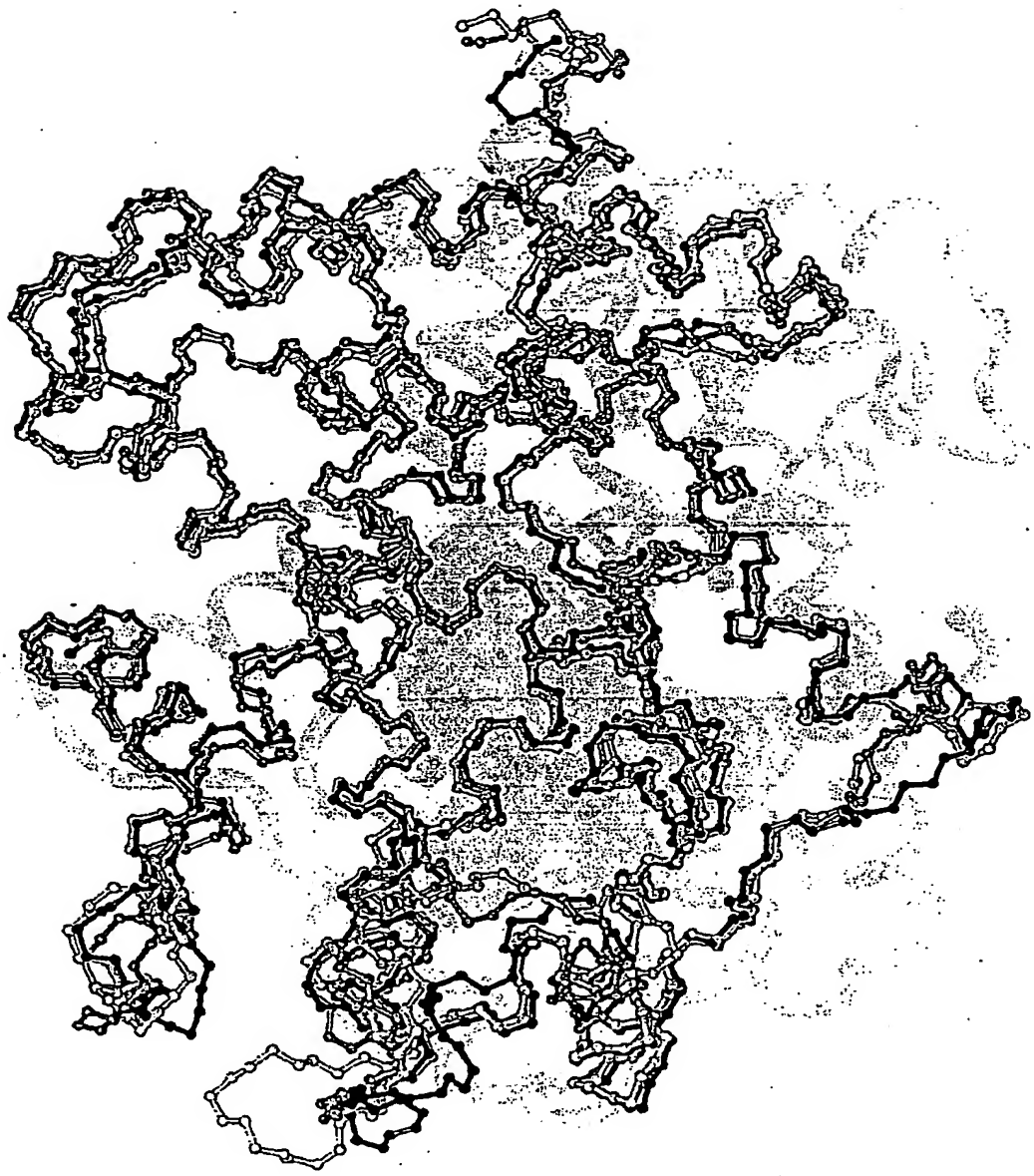

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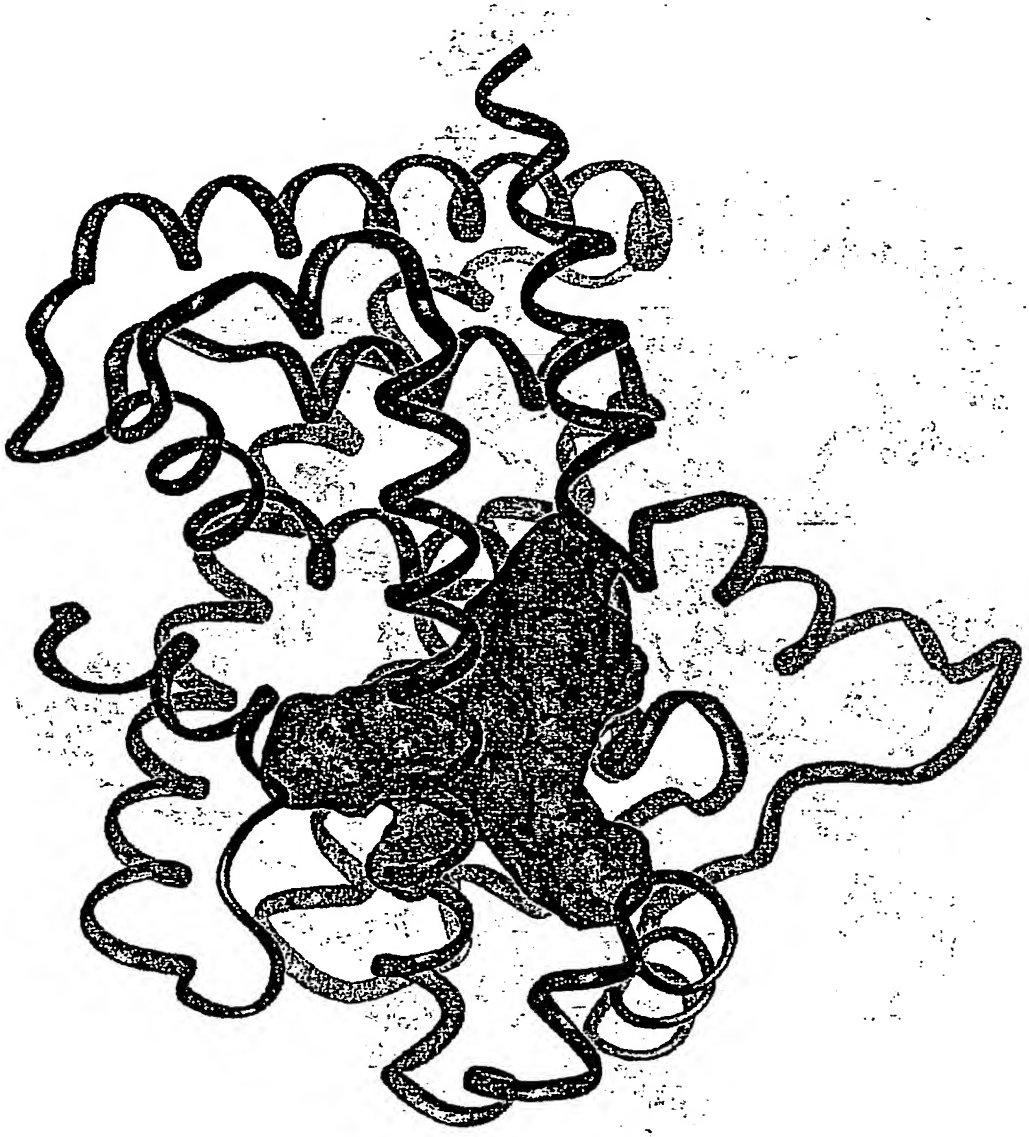

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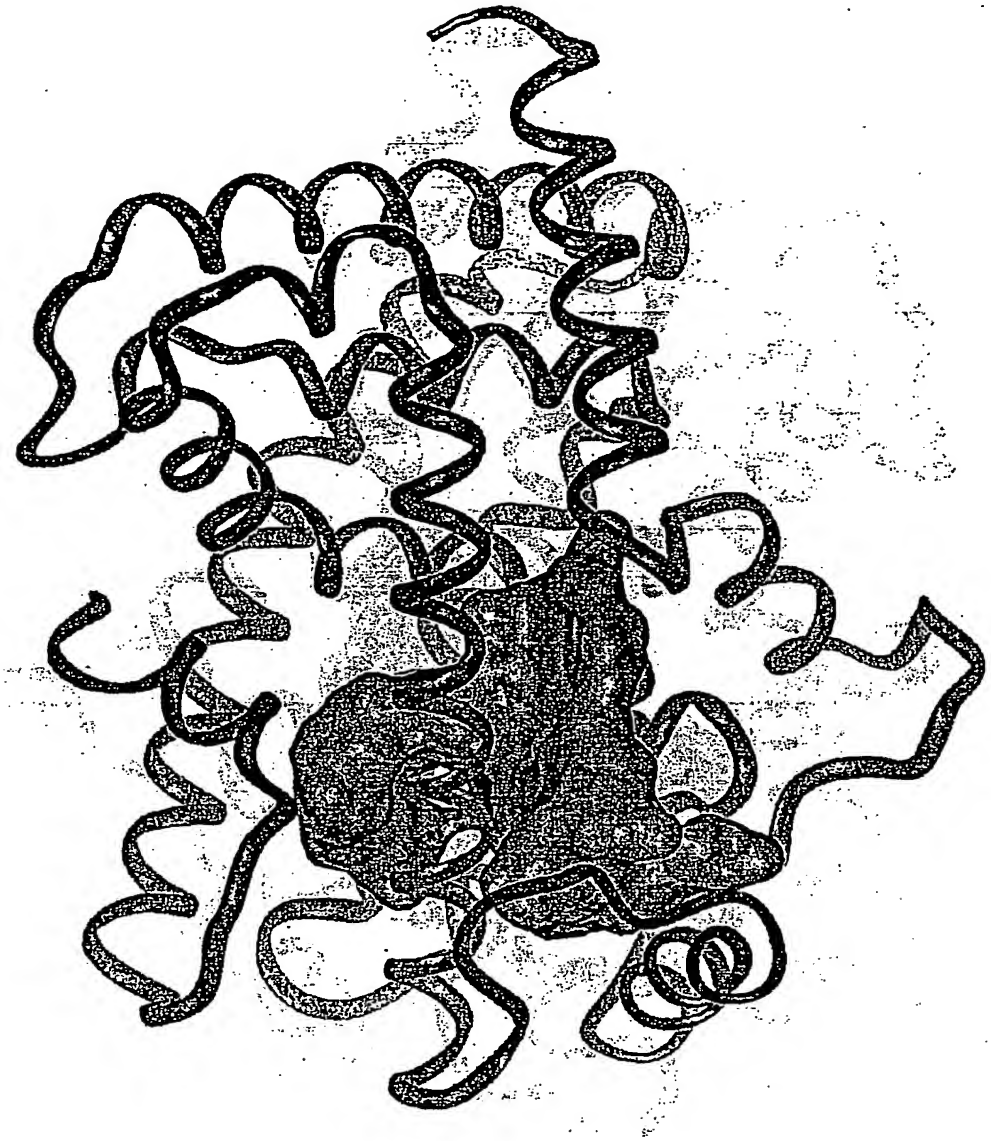

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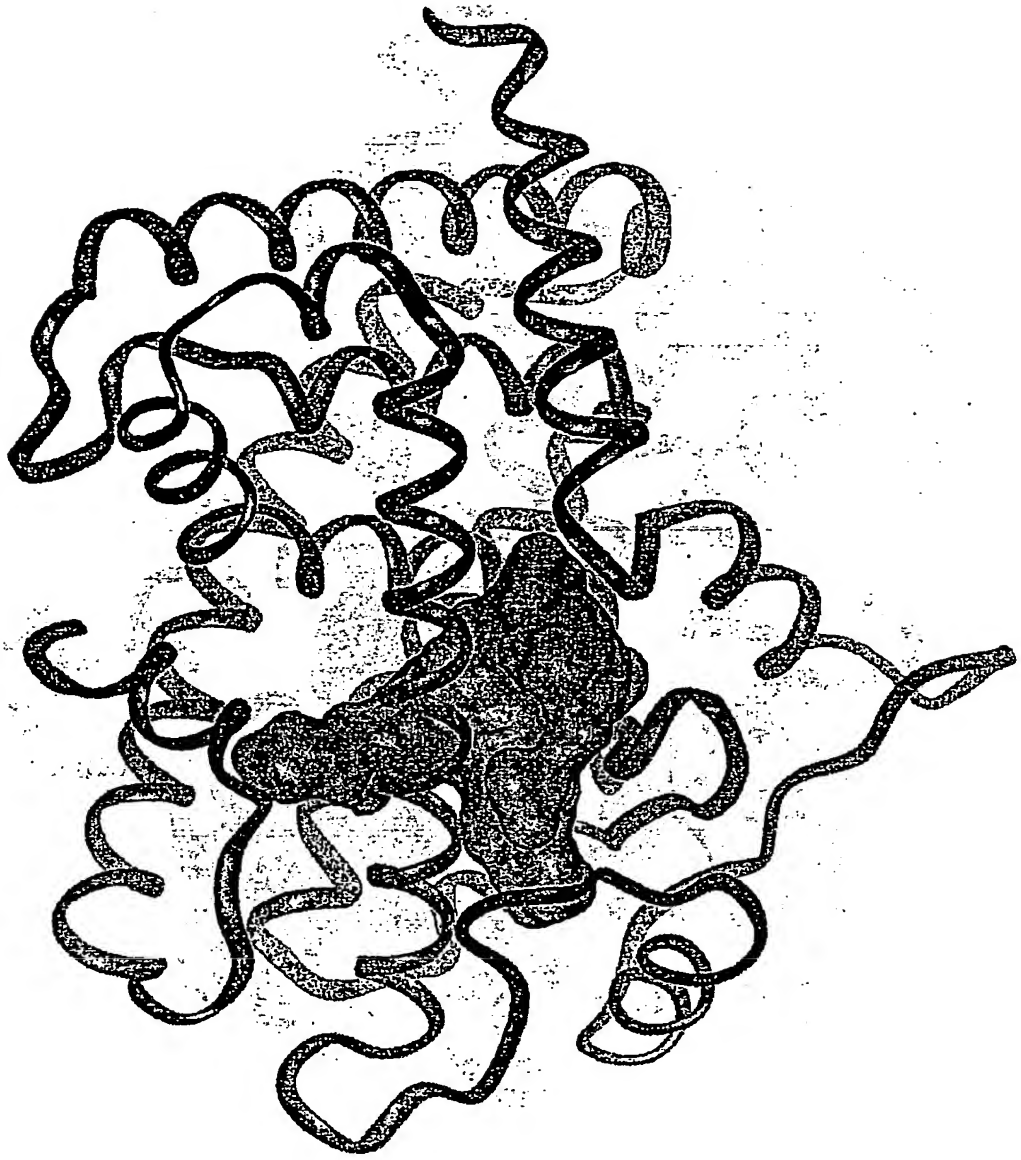

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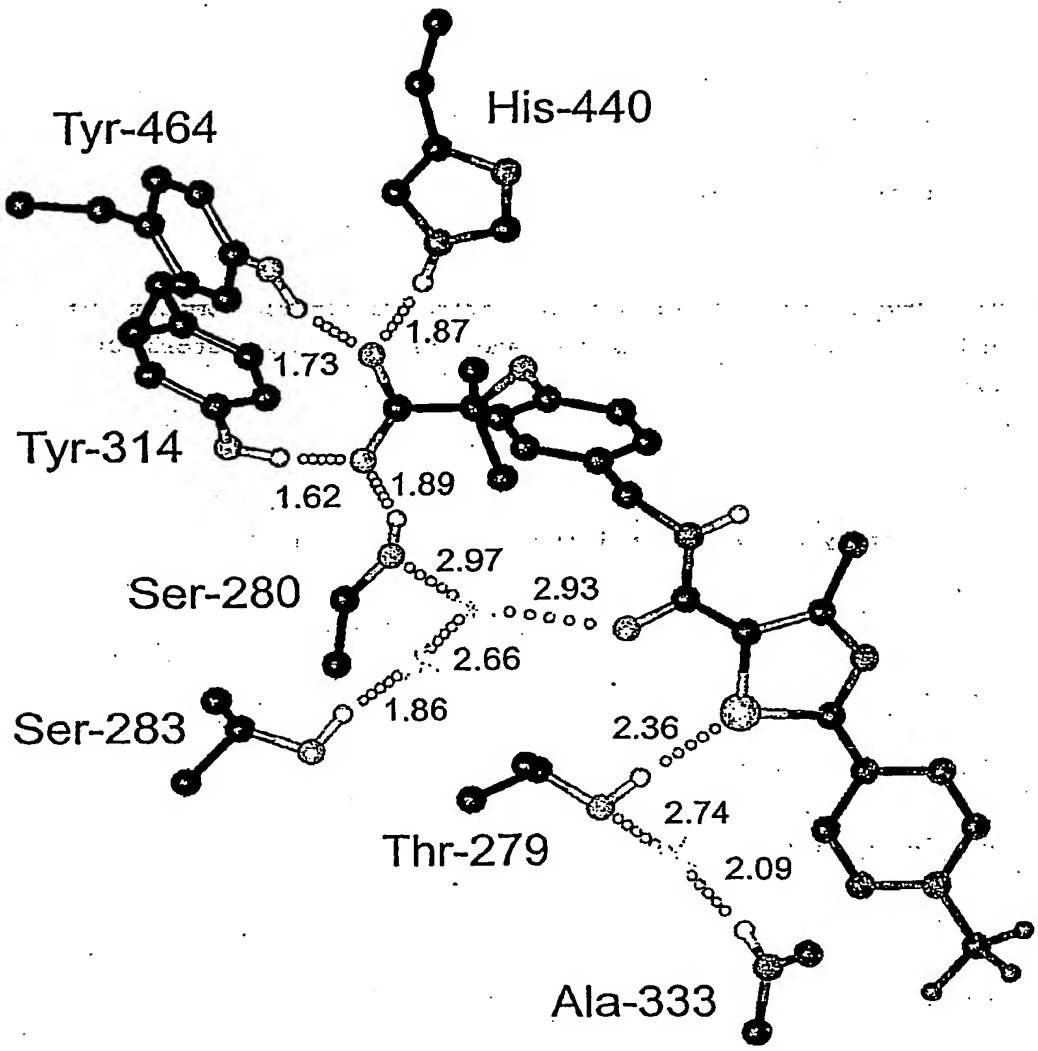

FIGURE 7

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Xu, Dr. Eric
Montana, Valerie
Lambert, Dr. Millard

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atgggaacca ccctgtagag gtccatctgc gttcagaccc agacgatgcc agagctatga    300

ctgggcctgc aggtgtggcg ccgaggggag atcagcc atg gag cag cca cag gag     355
                                          Met Glu Gln Pro Gln Glu
                                          1               5

gaa gcc cct gag gtc cgg gaa gag gag gag aaa gag gaa gtg gca gag      403
Glu Ala Pro Glu Val Arg Glu Glu Glu Glu Lys Glu Glu Val Ala Glu
            10                  15                  20

gca gaa gga gcc cca gag ctc aat ggg gga cca cag cat gca ctt cct      451
Ala Glu Gly Ala Pro Glu Leu Asn Gly Gly Pro Gln His Ala Leu Pro
        25                  30                  35

tcc agc agc tac aca gac ctc tcc cgg agc tcc tcg cca ccc tca ctg      499
Ser Ser Ser Tyr Thr Asp Leu Ser Arg Ser Ser Ser Pro Pro Ser Leu
    40                  45                  50

ctg gac caa ctg cag atg ggc tgt gac ggg gcc tca tgc ggc agc ctc      547
Leu Asp Gln Leu Gln Met Gly Cys Asp Gly Ala Ser Cys Gly Ser Leu
55                  60                  65                  70

aac atg gag tgc cgg gtg tgc ggg gac aag gca tcg ggc ttc cac tac      595
Asn Met Glu Cys Arg Val Cys Gly Asp Lys Ala Ser Gly Phe His Tyr
                75                  80                  85

ggt gtt cat gca tgt gag ggg tgc aag ggc ttc ttc cgt cgt acg atc      643
Gly Val His Ala Cys Glu Gly Cys Lys Gly Phe Phe Arg Arg Thr Ile
            90                  95                  100

cgc atg aag ctg gag tac gag aag tgt gag cgc agc tgc aag att cag      691
Arg Met Lys Leu Glu Tyr Glu Lys Cys Glu Arg Ser Cys Lys Ile Gln
        105                 110                 115

aag aag aac cgc aac aag tgc cag tac tgc cgc ttc cag aag tgc ctg      739
Lys Lys Asn Arg Asn Lys Cys Gln Tyr Cys Arg Phe Gln Lys Cys Leu
    120                 125                 130

gca ctg ggc atg tca cac aac gct atc cgt ttt ggt cgg atg ccg gag      787
Ala Leu Gly Met Ser His Asn Ala Ile Arg Phe Gly Arg Met Pro Glu
135                 140                 145                 150
gct gag aag agg aag ctg gtg gca ggg ctg act gca aac gag ggg agc      835
Ala Glu Lys Arg Lys Leu Val Ala Gly Leu Thr Ala Asn Glu Gly Ser
                155                 160                 165
```

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cag tac aac cca cag gtg gcc gac ctg aag gcc ttc tcc aag cac atc      883
Gln Tyr Asn Pro Gln Val Ala Asp Leu Lys Ala Phe Ser Lys His Ile
            170                 175                 180

tac aat gcc tac ctg aaa aac ttc aac atg acc aaa aag aag gcc cgc      931
Tyr Asn Ala Tyr Leu Lys Asn Phe Asn Met Thr Lys Lys Lys Ala Arg
        185                 190                 195

agc atc ctc acc ggc aaa gcc agc cac acg gcg ccc ttt gtg atc cac      979
Ser Ile Leu Thr Gly Lys Ala Ser His Thr Ala Pro Phe Val Ile His
    200                 205                 210

gac atc gag aca ttg tgg cag gca gag aag ggg ctg gtg tgg aag cag     1027
Asp Ile Glu Thr Leu Trp Gln Ala Glu Lys Gly Leu Val Trp Lys Gln
215                 220                 225                 230

ttg gtg aat ggc ctg cct ccc tac aag gag atc agc gtg cac gtc ttc     1075
Leu Val Asn Gly Leu Pro Pro Tyr Lys Glu Ile Ser Val His Val Phe
                235                 240                 245

tac cgc tgc cag tgc acc aca gtg gag acc gtg cgg gag ctc act gag     1123
Tyr Arg Cys Gln Cys Thr Thr Val Glu Thr Val Arg Glu Leu Thr Glu
            250                 255                 260

ttc gcc aag agc atc ccc agc ttc agc agc ctc ttc ctc aac gac cag     1171
Phe Ala Lys Ser Ile Pro Ser Phe Ser Ser Leu Phe Leu Asn Asp Gln
        265                 270                 275

gtt acc ctt ctc aag tat ggc gtg cac gag gcc atc ttc gcc atg ctg     1219
Val Thr Leu Leu Lys Tyr Gly Val His Glu Ala Ile Phe Ala Met Leu
    280                 285                 290

gcc tct atc gtc aac aag gac ggg ctg ctg gta gcc aac ggc agt ggc     1267
Ala Ser Ile Val Asn Lys Asp Gly Leu Leu Val Ala Asn Gly Ser Gly
295                 300                 305                 310

ttt gtc acc cgt gag ttc ctg cgc agc ctc cgc aaa ccc ttc agt gat     1315
Phe Val Thr Arg Glu Phe Leu Arg Ser Leu Arg Lys Pro Phe Ser Asp
                315                 320                 325

atc att gag cct aag ttt gaa ttt gct gtc aag ttc aac gcc ctg gaa     1363
Ile Ile Glu Pro Lys Phe Glu Phe Ala Val Lys Phe Asn Ala Leu Glu
```

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            330                 335                 340

ctt gat gac agt gac ctg gcc cta ttc att gcg gcc atc att ctg tgt    1411
Leu Asp Asp Ser Asp Leu Ala Leu Phe Ile Ala Ala Ile Ile Leu Cys
        345                 350                 355

gga gac cgg cca ggc ctc atg aac gtt cca cgg gtg gag gct atc cag    1459
Gly Asp Arg Pro Gly Leu Met Asn Val Pro Arg Val Glu Ala Ile Gln
    360                 365                 370

gac acc atc ctg cgt gcc ctc gaa ttc cac ctg cag gcc aac cac cct    1507
Asp Thr Ile Leu Arg Ala Leu Glu Phe His Leu Gln Ala Asn His Pro
375                 380                 385                 390

gat gcc cag tac ctc ttc ccc aag ctg ctg cag aag atg gct gac ctg    1555
Asp Ala Gln Tyr Leu Phe Pro Lys Leu Leu Gln Lys Met Ala Asp Leu
                395                 400                 405

cgg caa ctg gtc acc gag cac gcc cag atg atg cag cgg atc aag aag    1603
Arg Gln Leu Val Thr Glu His Ala Gln Met Met Gln Arg Ile Lys Lys
            410                 415                 420

acc gaa acc gag acc tcg ctg cac cct ctg ctc cag gag atc tac aag    1651
Thr Glu Thr Glu Thr Ser Leu His Pro Leu Leu Gln Glu Ile Tyr Lys
        425                 430                 435

gac atg tac taacggcggc acccaggcct ccctgcagac tccaatgggg            1700
Asp Met Tyr
    440

ccagcactgg aggggcccac ccacatgact tttccattga ccagctctct tcctgtcttt  1760

gttgtctccc tctttctcag ttcctctttc ttttctaatt cctgttgctc tgtttcttcc  1820

tttctgtagg tttctctctt cccttctccc ttctcccttg ccctcccttt ctctctccta  1880

tccccacgtc tgtcctcctt tcttattctg tgagatgttt tgtattattt caccagcagc  1940

atagaacagg acctctgctt ttgcacacct tttccccagg agcagaagag agtgggcctg  2000

ccctctgccc catcattgca cctgcaggct taggtcctca cttctgtctc ctgtcttcag  2060

agcaaaagac ttgagccatc caaagaaaca ctaagctctc tgggcctggg ttccagggaa  2120
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ggctaagcat ggcctggact gactgcagcc ccctatagtc atggggtccc tgctgcaaag 2180

gacagtggca gaccccggca gtagagccga gatgcctccc caagactgtc attgcccctc 2240

cgatcgtgag gccacccact gacccaatga tcctctccag cagcacacct cagccccact 2300

gacacccagt gtccttccat cttcacactg gtttgccagg ccaatgttgc tgatggcccc 2360

tccagcacac acacataagc actgaaatca ctttacctgc aggcaccatg cacctccctt 2420

ccctccctga ggcaggtgag aacccagaga gaggggcctg caggtgagca ggcagggctg 2480

ggccaggtct ccggggaggc aggggtcctg caggtcctgg tgggtcagcc cagcacctcg 2540

cccagtggga gcttcccggg ataaactgag cctgttcatt ctgatgtcca tttgtcccaa 2600

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atgccatgtc tgagcggcgc agagccctcc aggcctgcag gggcaagggg ctggctggag 2840

tctcagagca cagaggtagg agaactgggg ttcaagccca ggcttcctgg gtcctgcctg 2900

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g 2961

<210> 6

<211> 441

<212> PRT

<213> Homo sapiens

<400> 6

Met Glu Gln Pro Gln Glu Glu Ala Pro Glu Val Arg Glu Glu Glu Glu
1 5 10 15

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Lys Glu Glu Val Ala Glu Ala Glu Gly Ala Pro Glu Leu Asn Gly Gly
          20                  25                  30

Pro Gln His Ala Leu Pro Ser Ser Ser Tyr Thr Asp Leu Ser Arg Ser
        35                  40                  45

Ser Ser Pro Pro Ser Leu Leu Asp Gln Leu Gln Met Gly Cys Asp Gly
    50                  55                  60

Ala Ser Cys Gly Ser Leu Asn Met Glu Cys Arg Val Cys Gly Asp Lys
65                  70                  75                  80

Ala Ser Gly Phe His Tyr Gly Val His Ala Cys Glu Gly Cys Lys Gly
                85                  90                  95

Phe Phe Arg Arg Thr Ile Arg Met Lys Leu Glu Tyr Glu Lys Cys Glu
            100                 105                 110

Arg Ser Cys Lys Ile Gln Lys Lys Asn Arg Asn Lys Cys Gln Tyr Cys
        115                 120                 125

Arg Phe Gln Lys Cys Leu Ala Leu Gly Met Ser His Asn Ala Ile Arg
    130                 135                 140

Phe Gly Arg Met Pro Glu Ala Glu Lys Arg Lys Leu Val Ala Gly Leu
145                 150                 155                 160

Thr Ala Asn Glu Gly Ser Gln Tyr Asn Pro Gln Val Ala Asp Leu Lys
                165                 170                 175

Ala Phe Ser Lys His Ile Tyr Asn Ala Tyr Leu Lys Asn Phe Asn Met
            180                 185                 190

Thr Lys Lys Lys Ala Arg Ser Ile Leu Thr Gly Lys Ala Ser His Thr
        195                 200                 205

Ala Pro Phe Val Ile His Asp Ile Glu Thr Leu Trp Gln Ala Glu Lys
    210                 215                 220
```

```
Gly Leu Val Trp Lys Gln Leu Val Asn Gly Leu Pro Pro Tyr Lys Glu
225                 230                 235                 240

Ile Ser Val His Val Phe Tyr Arg Cys Gln Cys Thr Thr Val Glu Thr
                245                 250                 255

Val Arg Glu Leu Thr Glu Phe Ala Lys Ser Ile Pro Ser Phe Ser Ser
            260                 265                 270

Leu Phe Leu Asn Asp Gln Val Thr Leu Leu Lys Tyr Gly Val His Glu
        275                 280                 285

Ala Ile Phe Ala Met Leu Ala Ser Ile Val Asn Lys Asp Gly Leu Leu
    290                 295                 300

Val Ala Asn Gly Ser Gly Phe Val Thr Arg Glu Phe Leu Arg Ser Leu
305                 310                 315                 320

Arg Lys Pro Phe Ser Asp Ile Ile Glu Pro Lys Phe Glu Phe Ala Val
                325                 330                 335

Lys Phe Asn Ala Leu Glu Leu Asp Asp Ser Asp Leu Ala Leu Phe Ile
            340                 345                 350

Ala Ala Ile Ile Leu Cys Gly Asp Arg Pro Gly Leu Met Asn Val Pro
        355                 360                 365

Arg Val Glu Ala Ile Gln Asp Thr Ile Leu Arg Ala Leu Glu Phe His
    370                 375                 380

Leu Gln Ala Asn His Pro Asp Ala Gln Tyr Leu Phe Pro Lys Leu Leu
385                 390                 395                 400

Gln Lys Met Ala Asp Leu Arg Gln Leu Val Thr Glu His Ala Gln Met
                405                 410                 415
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Met Gln Arg Ile Lys Lys Thr Glu Thr Glu Thr Ser Leu His Pro Leu
420 425 430

Leu Gln Glu Ile Tyr Lys Asp Met Tyr
435 440

<210> 7

<211> 825

<212> DNA

<213> Homo sapiens

<220>

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Gln Tyr Asn Pro Gln Val Ala Asp Leu Lys Ala Phe Ser Lys His Ile
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tac aat gcc tac ctg aaa aac ttc aac atg acc aaa aag aag gcc cgc 96
Tyr Asn Ala Tyr Leu Lys Asn Phe Asn Met Thr Lys Lys Lys Ala Arg
20 25 30

agc atc ctc acc ggc aaa gcc agc cac acg gcg ccc ttt gtg atc cac 144
Ser Ile Leu Thr Gly Lys Ala Ser His Thr Ala Pro Phe Val Ile His
35 40 45

gac atc gag aca ttg tgg cag gca gag aag ggg ctg gtg tgg aag cag 192
Asp Ile Glu Thr Leu Trp Gln Ala Glu Lys Gly Leu Val Trp Lys Gln

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    50                  55                  60

ttg gtg aat ggc ctg cct ccc tac aag gag atc agc gtg cac gtc ttc      240
Leu Val Asn Gly Leu Pro Pro Tyr Lys Glu Ile Ser Val His Val Phe
65                  70                  75                  80

tac cgc tgc cag tgc acc aca gtg gag acc gtg cgg gag ctc act gag      288
Tyr Arg Cys Gln Cys Thr Thr Val Glu Thr Val Arg Glu Leu Thr Glu
                85                  90                  95

ttc gcc aag agc atc ccc agc ttc agc agc ctc ttc ctc aac gac cag      336
Phe Ala Lys Ser Ile Pro Ser Phe Ser Ser Leu Phe Leu Asn Asp Gln
            100                 105                 110

gtt acc ctt ctc aag tat ggc gtg cac gag gcc atc ttc gcc atg ctg      384
Val Thr Leu Leu Lys Tyr Gly Val His Glu Ala Ile Phe Ala Met Leu
        115                 120                 125

gcc tct atc gtc aac aag gac ggg ctg ctg gta gcc aac ggc agt ggc      432
Ala Ser Ile Val Asn Lys Asp Gly Leu Leu Val Ala Asn Gly Ser Gly
    130                 135                 140

ttt gtc acc cgt gag ttc ctg cgc agc ctc cgc aaa ccc ttc agt gat      480
Phe Val Thr Arg Glu Phe Leu Arg Ser Leu Arg Lys Pro Phe Ser Asp
145                 150                 155                 160

atc att gag cct aag ttt gaa ttt gct gtc aag ttc aac gcc ctg gaa      528
Ile Ile Glu Pro Lys Phe Glu Phe Ala Val Lys Phe Asn Ala Leu Glu
                165                 170                 175

ctt gat gac agt gac ctg gcc cta ttc att gcg gcc atc att ctg tgt      576
Leu Asp Asp Ser Asp Leu Ala Leu Phe Ile Ala Ala Ile Ile Leu Cys
            180                 185                 190

gga gac cgg cca ggc ctc atg aac gtt cca cgg gtg gag gct atc cag      624
Gly Asp Arg Pro Gly Leu Met Asn Val Pro Arg Val Glu Ala Ile Gln
        195                 200                 205

gac acc atc ctg cgt gcc ctc gaa ttc cac ctg cag gcc aac cac cct      672
Asp Thr Ile Leu Arg Ala Leu Glu Phe His Leu Gln Ala Asn His Pro
    210                 215                 220
gat gcc cag tac ctc ttc ccc aag ctg ctg cag aag atg gct gac ctg      720
Asp Ala Gln Tyr Leu Phe Pro Lys Leu Leu Gln Lys Met Ala Asp Leu
225                 230                 235                 240
```

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cgg caa ctg gtc acc gag cac gcc cag atg atg cag cgg atc aag aag      768
Arg Gln Leu Val Thr Glu His Ala Gln Met Met Gln Arg Ile Lys Lys
                245                 250                 255

acc gaa acc gag acc tcg ctg cac cct ctg ctc cag gag atc tac aag      816
Thr Glu Thr Glu Thr Ser Leu His Pro Leu Leu Gln Glu Ile Tyr Lys
            260                 265                 270

gac atg tac                                                          825
Asp Met Tyr
        275
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<210> 8

<211> 275

<212> PRT

<213> Homo sapiens

<400> 8

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Gln Tyr Asn Pro Gln Val Ala Asp Leu Lys Ala Phe Ser Lys His Ile
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Tyr Asn Ala Tyr Leu Lys Asn Phe Asn Met Thr Lys Lys Lys Ala Arg
            20                  25                  30

Ser Ile Leu Thr Gly Lys Ala Ser His Thr Ala Pro Phe Val Ile His
        35                  40                  45

Asp Ile Glu Thr Leu Trp Gln Ala Glu Lys Gly Leu Val Trp Lys Gln
    50                  55                  60

Leu Val Asn Gly Leu Pro Pro Tyr Lys Glu Ile Ser Val His Val Phe
65                  70                  75                  80
```

```
Tyr Arg Cys Gln Cys Thr Thr Val Glu Thr Val Arg Glu Leu Thr Glu
                85                  90                  95

Phe Ala Lys Ser Ile Pro Ser Phe Ser Ser Leu Phe Leu Asn Asp Gln
            100                 105                 110

Val Thr Leu Leu Lys Tyr Gly Val His Glu Ala Ile Phe Ala Met Leu
        115                 120                 125

Ala Ser Ile Val Asn Lys Asp Gly Leu Leu Val Ala Asn Gly Ser Gly
    130                 135                 140

Phe Val Thr Arg Glu Phe Leu Arg Ser Leu Arg Lys Pro Phe Ser Asp
145                 150                 155                 160

Ile Ile Glu Pro Lys Phe Glu Phe Ala Val Lys Phe Asn Ala Leu Glu
                165                 170                 175

Leu Asp Asp Ser Asp Leu Ala Leu Phe Ile Ala Ala Ile Ile Leu Cys
            180                 185                 190

Gly Asp Arg Pro Gly Leu Met Asn Val Pro Arg Val Glu Ala Ile Gln
        195                 200                 205

Asp Thr Ile Leu Arg Ala Leu Glu Phe His Leu Gln Ala Asn His Pro
    210                 215                 220

Asp Ala Gln Tyr Leu Phe Pro Lys Leu Leu Gln Lys Met Ala Asp Leu
225                 230                 235                 240

Arg Gln Leu Val Thr Glu His Ala Gln Met Met Gln Arg Ile Lys Lys
                245                 250                 255

Thr Glu Thr Glu Thr Ser Leu His Pro Leu Leu Gln Glu Ile Tyr Lys
            260                 265                 270

Asp Met Tyr
        275
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<210> 9

<211> 11

<212> PRT

<213> Artificial Purification Sequence

<400> 9

Met Lys Lys Gly His His His His His His Gly
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